National Aeronautics and Space Administration

HIGH-END COMPUTING CAPABILITY PORTFOLIO

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NASA Advanced Supercomputing Division

February 10, 2020

Coordinating Early User Access to Aitken Expansion Increases Utilization

- HECC's Application Performance and Productivity (APP) team coordinated user access to test the Aitken expansion racks, overlapping with APP activities that would normally have exclusive access. High demand for HECC resources motivates looking for ways to get science and engineering jobs onto the expansion nodes as soon as possible.
- APP staff and HECC management worked with the HECC Security team to allow access to a few selected users who have NASA PIV badges before completion of the Security Impact Analysis (SIA) of the resources.
- The APP team performed some basic functionality tests, installed compilers and MPI libraries, and started performance characterization and SBU rate measurement; and added a small number of users to help with testing.
  - Users tailored their build scripts and did performance tuning.
  - Both groups found configuration issues, such as stale password files on the compute nodes and problems with automounting filesystems, which the HECC Systems team fixed.
- After the system became more stable, additional users were given access to do production work before and during the SIA. When the SIA is complete, the system will go into "open early access," where all users can get on for testing before the system is moved into full production.

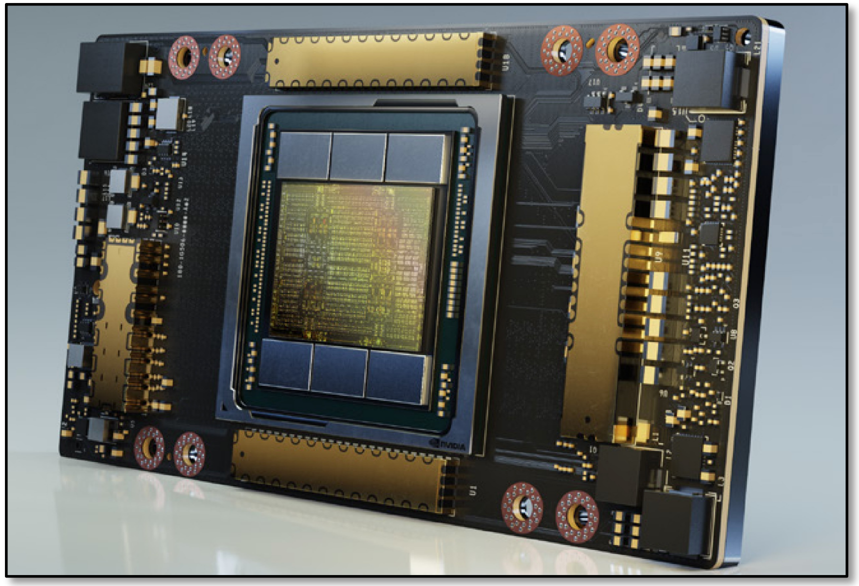
IMPACT: By overlapping system performance investigation with testing by a small number of users, HECC made productive use of machine cycles that would otherwise have gone unused.

The eight racks of the Aitken expansion provide 1,024 AMD EPYC 7742 Rome nodes with 128 cores per node. With 131,072 cores, the expansion has more total cores than the entire Electra system.
Matt Lepp, Unisys

Evaluation of A100 GPUs in Amazon Cloud Shows Promising Results

- As part of investigations into pathfinding systems that might be suitable for future HECC procurements, the Applications Performance and Productivity (APP) team recently started using Amazon Web Services (AWS) to evaluate NVIDIA A100 GPUs.
- For HPC applications, the A100s are touted to be up to 2 times faster than the current V100s on site at the NAS facility, making the A100 a candidate for future HECC procurements.
- In December 2020, the HECC Cloud team added A100-equipped nodes at AWS to its capability, and the APP team started a comparison with the on-premises V100s.
- Preliminary results are encouraging:
  - Except for the embarrassingly parallel kernel, the OpenACC version of the NAS Parallel Benchmarks showed a performance increase ranging between 14% and 157% compared to the V100.
  - The kernels of Eddy, a CFD code, showed improvements of 40–60%.
  - The GPU kernels of the Aladyn molecular dynamics mini-application showed improvements of 20–60%.
- The next step is to compare the performance of some machine learning applications.

IMPACT: The ability to evaluate cloud-based resources helps HECC appraise new computer architectures early in their life cycle and reduces risk in future procurements of production systems.

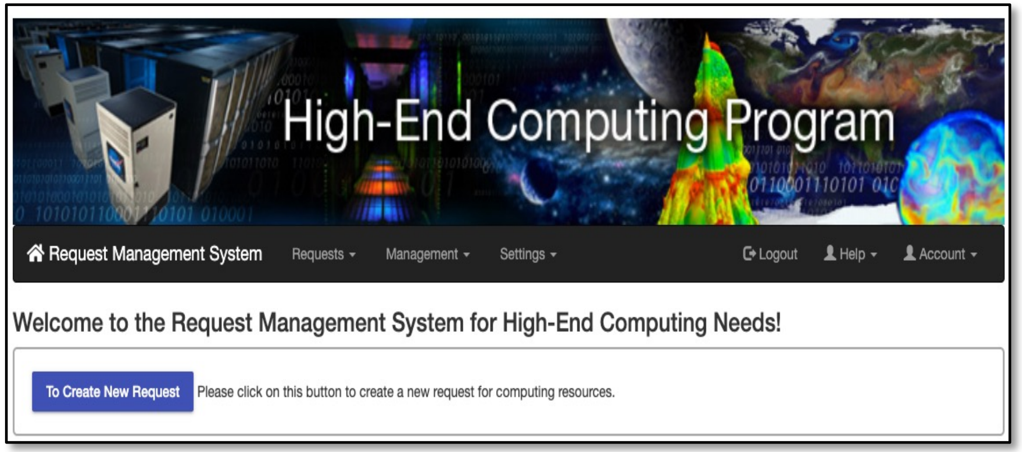


The NVIDIA A100 Tensor Core GPU provides acceleration for AI, data analytics, and HPC. It can be partitioned into seven GPU instances to dynamically adjust to shifting demands.
Image courtesy of NVIDIA

Resource Management System Version 1.3 Released

- HECC, in collaboration with NASA Center for Climate Simulation (NCCS), released version 1.3 of the Request Management System (RMS) on January 5, 2021. This tool is being developed to replace REI eBooks.
- While RMS currently only supports the Science Mission Directorate (SMD), the Board of Advisors have approved integration of the other mission directorates in version 1.4.
- Completion of this milestone concluded the third phase of a multi-phase collaboration.
- Version 1.3 new features include:
  - Generating exportable reports by fiscal year.
  - Generating exportable reports for funding confirmation, allocation, and modification.
  - Enabling bulk allocation through Excel, rather than doing each allocation by hand.
- These new features will become available to all mission directorates when version 1.4 is released in late February 2021.

IMPACT: Creating in-house-developed software to manage supercomputer resource allocation requests allows NASA's High End Computing Program more ownership of the data and simplifies the process for reviewing allocations and targets.

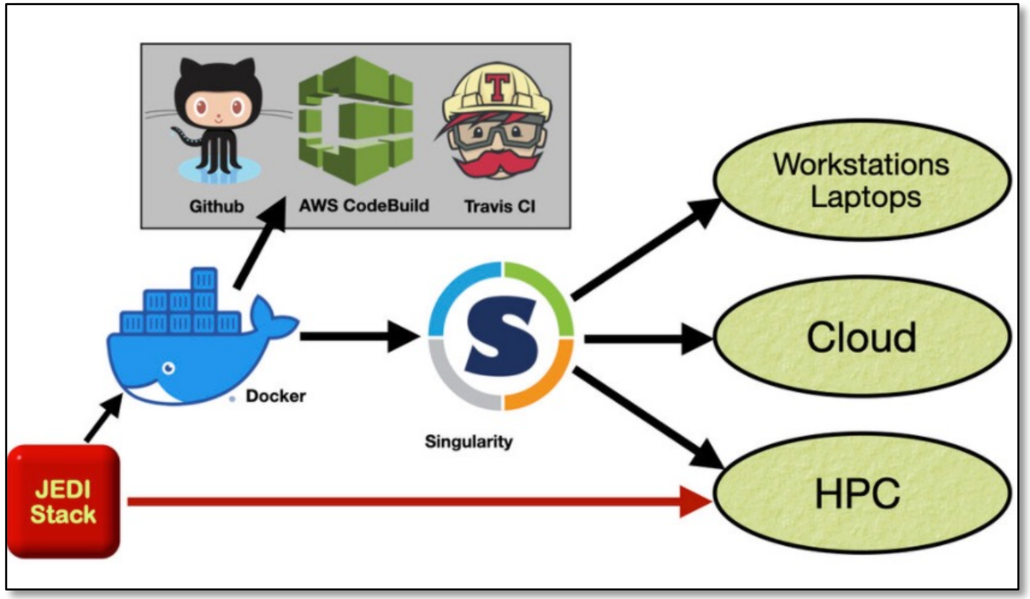


Snapshot of the welcome page for the Request Management System.

JEDI Containers Successfully Ported to HECC Resources

- Engineers on the Application Performance and Productivity (APP) team successfully ported and ran high-performance Singularity containers from the Joint Effort for Data assimilation Integration (JEDI) project of the Joint Center for Satellite Data Assimilation (JCSDA) on both HECC in-house and AWS Cloud resources.
  - Two JEDI containers and a test case to run a three-dimensional variational data assimilation application (3DVar) with resolution c192 (~50 km) using 864 MPI ranks were provided by JEDI developer, Mark Miesch.
- Both containers, differing in whether the Mellanox drivers are included, ran across multiple nodes with run times of 19 to 30 minutes on various HECC in-house processor types with one caveat:
  - HECC's Skylake and Cascade Lake nodes are divided into A blades and B blades, where their InfiniBand interfaces (ib0 and ib1) are on opposite subnets.
  - Running the container without the Mellanox drivers on Skylake and Cascade Lake requires an additional setting of FI_PROVIDER=sockets (26 min) or using only nodes whose ib0 are on the same subnet (19 min).
- On AWS cloud, after troubleshooting system configuration and filesystem issues, the containers ran with runtimes of 14 to 26 minutes.
- APP's experiences in porting these containers will help a NASA Goddard scientist who wants to use them on HECC resources.

IMPACT: Use of high-performance Singularity JEDI containers saves time and effort for NASA scientists engaged in operational weather forecasting using HECC and cloud resources.

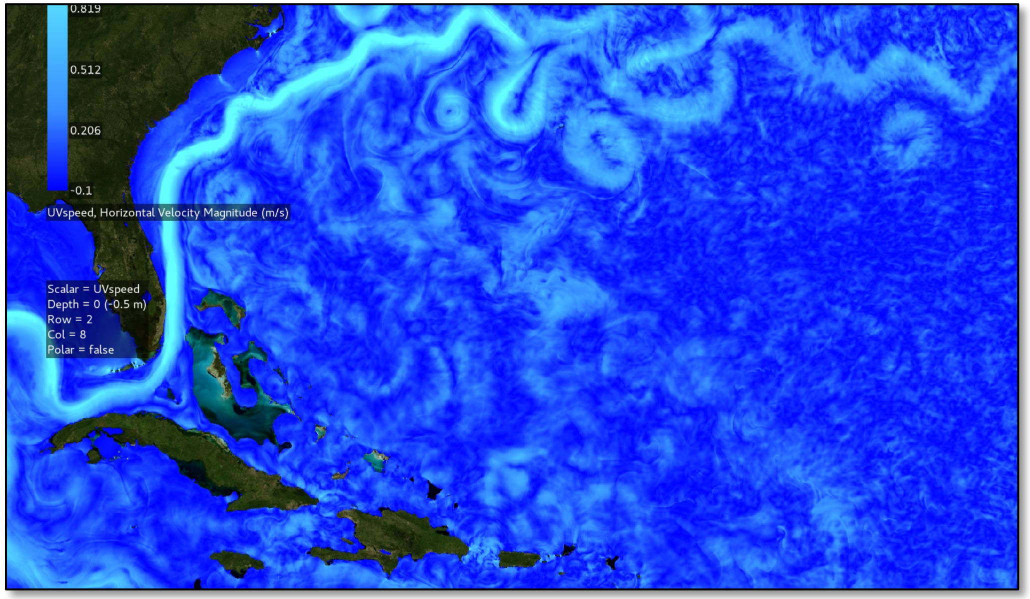


The JEDI container workflow and JEDI-stack build system. *Image borrowed with permission from Mark Miesch's publication "JEDI to GO: High-Performance Containers for Earth System Prediction."*

Application Experts Improve Performance of Ocean Code

- HECC's Applications Performance and Productivity (APP) team recently improved the performance of the Massachusetts Institute of Technology General Circulation Model (MITgcm) by 12–124%, depending on the model configuration.
  - MITgcm simulates circulation of ocean currents over a wide range of scales (from hundreds of kilometers down to hundreds of meters).
  - Several projects use MITgcm on HECC resources. The code was the 10th-most heavily used application for HECC in FY20.
- The APP team used a variety of tools to locate bottlenecks, combined with their in-depth knowledge of the HECC environment and hardware, to implement solutions to those bottlenecks.
  - The primary benefit resulted from making appropriate compile-time choices of the conditional code paths, where performance improvement in production will require only rebuilding the executable.
  - Further benefits resulted from an extensive rework of filesystem usage, and optimization of seven computational routines.
- The APP team's findings were presented to the users and were well received. They will continue working with users, as the MITgcm community has asked for further assistance in analyzing their workflows.

IMPACT: Performance improvements for heavily used codes such as MITgcm decrease the time to solution for the user and free system resources for other work.

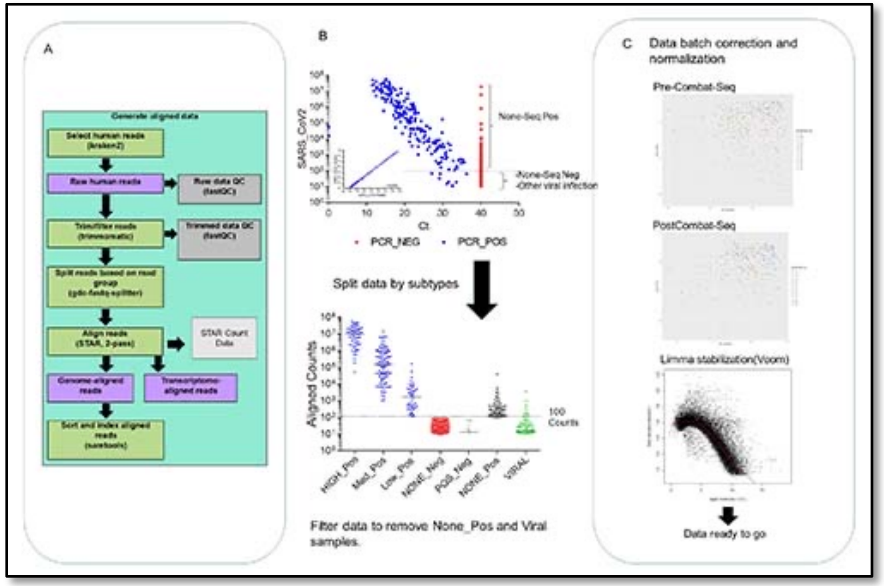


A visualization highlighting the Gulf Stream showing near-surface water speed from a 1/48-degree year-long global ocean simulation using MITgcm. *David Ellsworth, NASA/Ames*

Gene Hub Analysis Identifies Host Response to COVID-19 *

- As part of the COVID-19 International Research Team (COV-IRT), researchers from NASA Ames and around the country, working within the COVID 19 HPC Consortium, analyzed 845 samples (732 patient nasal swabs, 62 environmental swabs, and 51 control samples) in order to identify common co-expressed gene patterns that are related to the amount of SARS-CoV-2 viral particles in patients' blood.
- Results revealed a strong immune system response following SARS-CoV-2 infection.
  - Gene ontology analysis (topGO) of gene-hubs identified by weighted gene co-expression network analysis (WGCNA) of SARS-CoV-2 RNAseq expression data revealed a series of related biological pathways involving the innate immune system that are enriched in patients infected with SARS-CoV-2.
  - Analysis of RNA sequencing data showed that some samples that were negative for COVID-19 based on the nasal swab PCR test actually contained viral genomic matter based on identification of viral genomic material and host gene responses.
- Three data processing pipelines were established and optimized to enable the rapid alignment and analysis of the sequencing data using HECC resources and services.

IMPACT: HECC resources and services played a critical in role in generating the data for this COVID project, which is helping answer questions surrounding COVID-19, from basic science on how the virus interacts with cells in humans, to genetic risk factors to screening for potential therapeutic drugs.



COVID-19 RNAseq data analysis pipeline. *Robert Meller, Morehouse School of Medicine*

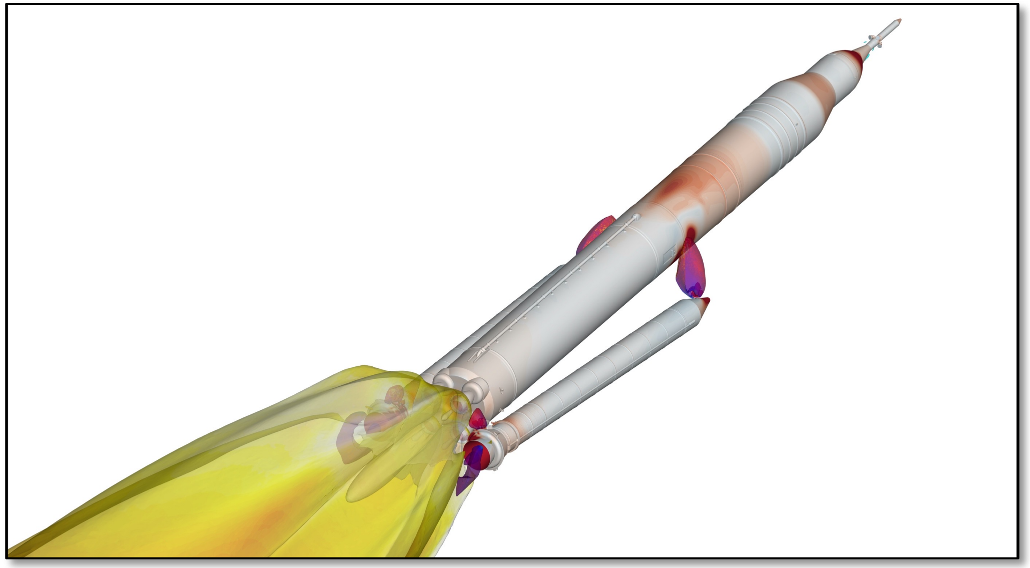
** HECC provided supercomputing resources and services in support of this work.*

Developing Booster Separation Databases for Artemis *

- In support of the Artemis Program, researchers at NASA Ames created detailed aerodynamic databases for the SLS solid-rocket booster (SRB) separation event using HECC resources. The conditions during the SRB separation phase of flight are difficult, if not impossible, to model in an experimental setting.
- Simulations were made using NASA's FUN3D and OVERFLOW CFD codes, modeling a total of 22 different rocket plumes and 13 independent variables. Thousands of data points were required in order to provide full coverage of the database.
- The databases will be used by the Guidance, Navigation, and Control group at NASA's Marshall Space Flight Center to model the separation event for Artemis missions and to ensure that the boosters can separate successfully without reconnecting the core under all possible flight conditions.
- This work was run on the Pleiades and Electra supercomputers, with each case using approximately 2,500 core hours. The nominal database required 5,780 FUN3D simulations, with an additional 13,000 supporting simulations.

** HECC provided supercomputing resources and services in support of this work.*

IMPACT: Enabled by HECC resources, these databases will be used to ensure that the Space Launch System's booster separation event occurs successfully, reducing the risk to crews of future Artemis missions to the lunar surface.



Isometric view of the Artemis booster separation event with the Block 1B variant of the Space Launch System. The vehicle surface is colored by pressure contours, where blue is low and red is high. Isosurfaces of high Mach number colored by temperature show the multiple rocket plumes modeled. *Jamie Meeroff, Derek Dalle, NASA/Ames*

Papers

- "**Dissipation Measures in Weakly-Collisional Plasmas**," O. Pezzi, et al., arXiv:2101.00722 [physics.plasm-ph], January 3, 2021. *
https://arxiv.org/abs/2101.00722
- "**Masses and Compositions of Three Small Planets Orbiting the Nearby M Dwarf L231-32 (TOI-270) and the M Dwarf Radius Valley**," V. Van Eylen, et al., arXiv:2101.01593 [astro-ph.EP], January 5, 2021. *
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- "**TESS Delivers Five New Hot Giant Planets Orbiting Bright Stars from the Full Frame Images**," J. Rodriguez, et al., arXiv:2101.01726 [astro-ph.EP], January 5, 2021. *
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- "**The Impact of Kinetic Neutrals on the Heliotail**," A. Michael, M. Opher, T. Toth, V. Tenishev, J. Drake, The Astrophysical Journal, vol. 906, no.1, published online Journal 5, 2021. *
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- "**TOI-1259Ab – A Gas Giant Planet with 2.7% Deep Transits and a Bound White Dwarf Companion**," D. Martin, et al., arXiv:2101.02707 [astro-ph.EP], January 7, 2021. *
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- "**TIC 168789840: A Sextuply-Eclipsing Sextuple Star System**," B. Powell, et al., arXiv:2101.03433 [astro-ph.SR], January 9, 2021. *
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Papers (cont.)

- **2021 AIAA SciTech Forum,** January 11-21, 2021, Virtual Event.
  - “**Rapid Aero Modeling for Urban Air Mobility Aircraft in Computational Experiments**,” P. Murphy, P. Buning, B. Simmons. *
    https://arc.aiaa.org/doi/abs/10.2514/6.2021-1002
  - “**Transition Analysis for the CRM-NLF Wind Tunnel Configuration**,” P. Paredes, et al. *
    https://arc.aiaa.org/doi/abs/10.2514/6.2021-1431
  - “**Improvements in Iterative Convergence of FUN3D Solutions**,” L. Wang, B. Diskin, E. Nielsen, Y. Liu. *
    https://arc.aiaa.org/doi/abs/10.2514/6.2021-0857
  - “**Verification Test Suite for Spalart-Allmaras QCR2000 Turbulence Model**,” B. Diskin, et al. *
    https://arc.aiaa.org/doi/abs/10.2514/6.2021-1552
  - “**Wall-Modeled LES of Flow over a Gaussian Bump**,” P. Iyer, M. Malik. *
    https://arc.aiaa.org/doi/abs/10.2514/6.2021-1438
  - “**A Computational Analysis of Boundary Layer Instability Over the BOLT Configuration**,” M. Choudhari, F. Li, P. Paredes. *
    https://arc.aiaa.org/doi/abs/10.2514/6.2021-1207
  - “**An Adjoint Elasticity Solver for High-Order Mesh Deformation**,” J. Marcon, A. Garai, M. Denison, S. Murman. *
    https://arc.aiaa.org/doi/abs/10.2514/6.2021-1238
  - “**Discontinuous Galerkin Simulations of Dusty Flows over a Full-Scale Capsule During Mars Atmospheric Entry**,” E. Ching, M. Ihme. *
    https://arc.aiaa.org/doi/abs/10.2514/6.2021-1518
  - “**Direct Numerical Simulation of Single-Species and Binary-Species Boundary Layers at High Pressure**,” T. Toki, J. Bellan. *
    https://arc.aiaa.org/doi/abs/10.2514/6.2021-0682

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Papers (cont.)

- **2021 AIAA SciTech Forum** (cont.)
  - “**Improvements in Simulating a Mach 0.80 Transonic Truss-Braced Wing Configuration Using the Spalart-Allmaras and k-ω SST Turbulence Models**,” D. Maldonado, et al. *
    https://arc.aiaa.org/doi/abs/10.2514/6.2021-1531
  - “**Pterodactyl: Aerodynamic and Aeroheating Model for a Symmetric Deployable Entry Vehicle with Flaps**,” B Reddish, et al. *
    https://arc.aiaa.org/doi/abs/10.2514/6.2021-0763
  - “**Structured Overset and Unstructured Grid Simulations for the Third AIAA Sonic Boom Prediction Workshop**,” J. Duensing, et al. *
    https://arc.aiaa.org/doi/abs/10.2514/6.2021-0471
  - “**Toward Numerical Investigation of Ignition and Combustion Transition in a Subscale LOX/Methane Rocket Combustor**,” M. Bonanni, et al. *
    https://arc.aiaa.org/doi/abs/10.2514/6.2021-1141
  - “**Design of a Crossflow Attenuated Natural Laminar Flow Flight Test Article**,” M. Lynde, R. Campbell, B. Hiller, L. Owens. *
    https://arc.aiaa.org/doi/abs/10.2514/6.2021-0173
  - “**High-Fidelity Simulations of HyMETS Arc-Jet Flows for PICA-N Modeling**,” P. Ventura Diaz, et al. *
    https://arc.aiaa.org/doi/abs/10.2514/6.2021-1629
  - “**Unstructured LES_DNS of a Turbulent Boundary Layer over a Gaussian Bump**,” J. Wright, R. Balin, K. Jansen, J. Evans. *
    https://arc.aiaa.org/doi/abs/10.2514/6.2021-1746
  - “**Direct Numerical Simulation of High-Pressure Free Jets**,” N. Sharan, J. Bellan. *
    https://arc.aiaa.org/doi/abs/10.2514/6.2021-0550
  - “**Hypersonic Second Mode Instability Response to Shaped Roughness**,” A. Leidy, R. King, M. Choudhari, P. Paredes. *
    https://arc.aiaa.org/doi/abs/10.2514/6.2021-0149

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Papers (cont.)

- **2021 AIAA SciTech Forum** (cont.)
  - ”**Surface-Normal Active Flow Control for Lift Enhancement and Separation Mitigation for High-Lift Common Research Model**,” S. Hosseini, C. Van Dam, S. Pandya. *
    https://arc.aiaa.org/doi/abs/10.2514/6.2021-1192
  - “**A High-Fidelity Coupling Framework for Aerothermoelastic Analysis and Adjoint-Based Gradient Evaluation**,” J. Smith, et al. *
    https://arc.aiaa.org/doi/abs/10.2514/6.2021-0407
  - “**Computational Design Methodology of Adaptive Outer Mold Line for Robust Low En-Route Noise of a Supersonic Aircraft**,” J. Weaver-Rosen, et al. *
    https://arc.aiaa.org/doi/abs/10.2514/6.2021-0877
  - “**Jet Noise Prediction with Large-Eddy Simulation for Chevron Nozzle Flows**,” G.-D. Stich, J. Housman, A. Ghate, C. Kiris. *
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  - “**Cartesian Mesh Simulations for the Third AIAA Sonic Boom Prediction Workshop**,” W. Spurlock, M. Aftosmis, M. Nemec. *
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  - “**Development of a Discontinuous Galerkin Solver Using Legion for Heterogeneous High-Performance Computing Architectures**,” K. Bando, S. Brill, E. Slaughter, M. Sekachev, A. Aiken, M. Ihme. *
    https://arc.aiaa.org/doi/abs/10.2514/6.2021-0140
  - “**CFD 2030 Grand Challenge: CFD-in-the-Loop Monte Carlo Flight Simulation for Space Vehicle Design**,” D. Schuster. *
    https://arc.aiaa.org/doi/abs/10.2514/6.2021-0957

- “**The TESS-Keck Survey. II. An Ultra-Short-Period Rocky Planet and Its Siblings Transiting the Galactic Thick-Disk Star TOI-561**,” L. Weiss, et al., The Astronomical Journal, vol. 161, no. 2, January 11, 2021. *
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Papers (cont.)

- "**A Hot Mini-Neptune in the Radius Valley Orbiting Solar Analogue HD 110113**," H. Osborn, et al., arXiv:2101.04745 [astro-ph.EP], January 12, 2021. *
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- "**High Order Nonlinear Filter Methods for Subsonic Turbulence Simulation with Stochastic Forcing**," A. Kritsuk, D. Kotov, B. Sjogreen, H. Yee, Journal of Computational Physics, published online January 13, 2021. *
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- "**TESS Hunt for Young and Maturing Exoplanets (THYME). IV. Three Small Planets Orbiting a 120 Myr Old Star in the Pisces-Eridanus Stream**," E. Newton, et al., The Astrophysical Journal, vol. 161, no. 2, January 14, 2021. *
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- "**Quantifying Scatter in Galaxy Formation at the Lowest Masses**," F. Munshi, A. Brooks, E. Applebaum, C. Christensen, J. Sligh, T. Quinn, arXiv:2101.05822 [astro-ph.GA], January 14, 2021. *
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- "**Development of a Physically-Informed Neural Network Interatomic Potential for Tantalum**," Y.-S. Lin, G. Purja Pun, Y. Mishin, arXiv:2101.06540 [cond-mat.mtrl-sci], January 16, 2021. *
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Papers (cont.)

- "**Automated Digital Elevation Model (DEM) Generation from Very-High-Resolution Planet SkySat Triplet Stereo and Video Imagery**," S. Bhushan, D. Shean, O. Alexandrov, S. Henderson, ISPRS Journal of Photogrammetry and Remote Sensing, vol. 173, published online January 22, 2021. *
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- "**An Explanation of the Nightside Ionospheric Structure of Venus**," S. Brecht, S. Ledvina, Journal of Geophysical Research: Space Physics, published online January 25, 2021. *
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- "**A Surface Mesh Deformation Method Near Component Intersections for High-Fidelity Design Optimization**," A. Yildirim, C. Mader, J. Martins, *Engineering with Computers* (Springer), published online January 27, 2021. *
https://link.springer.com/article/10.1007/s00366-020-01247-w
- "**Impacts of Saharan Mineral Dust on Air-Sea Interaction over North Atlantic Ocean Using a Fully Coupled Regional Model**," S.-H. Chen, et al., Journal of Geophysical Research: Atmospheres, published online January 27, 2021. *
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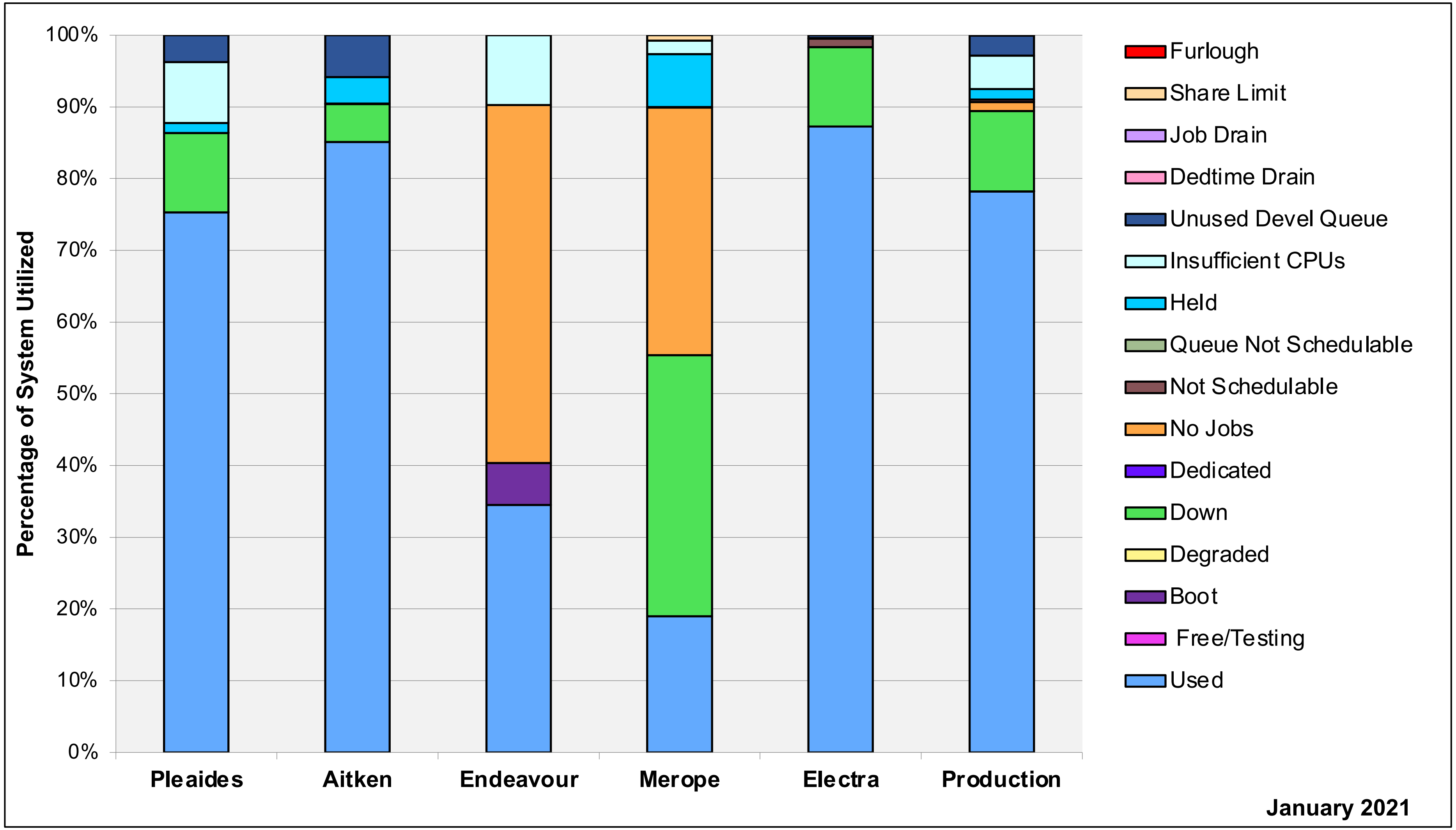
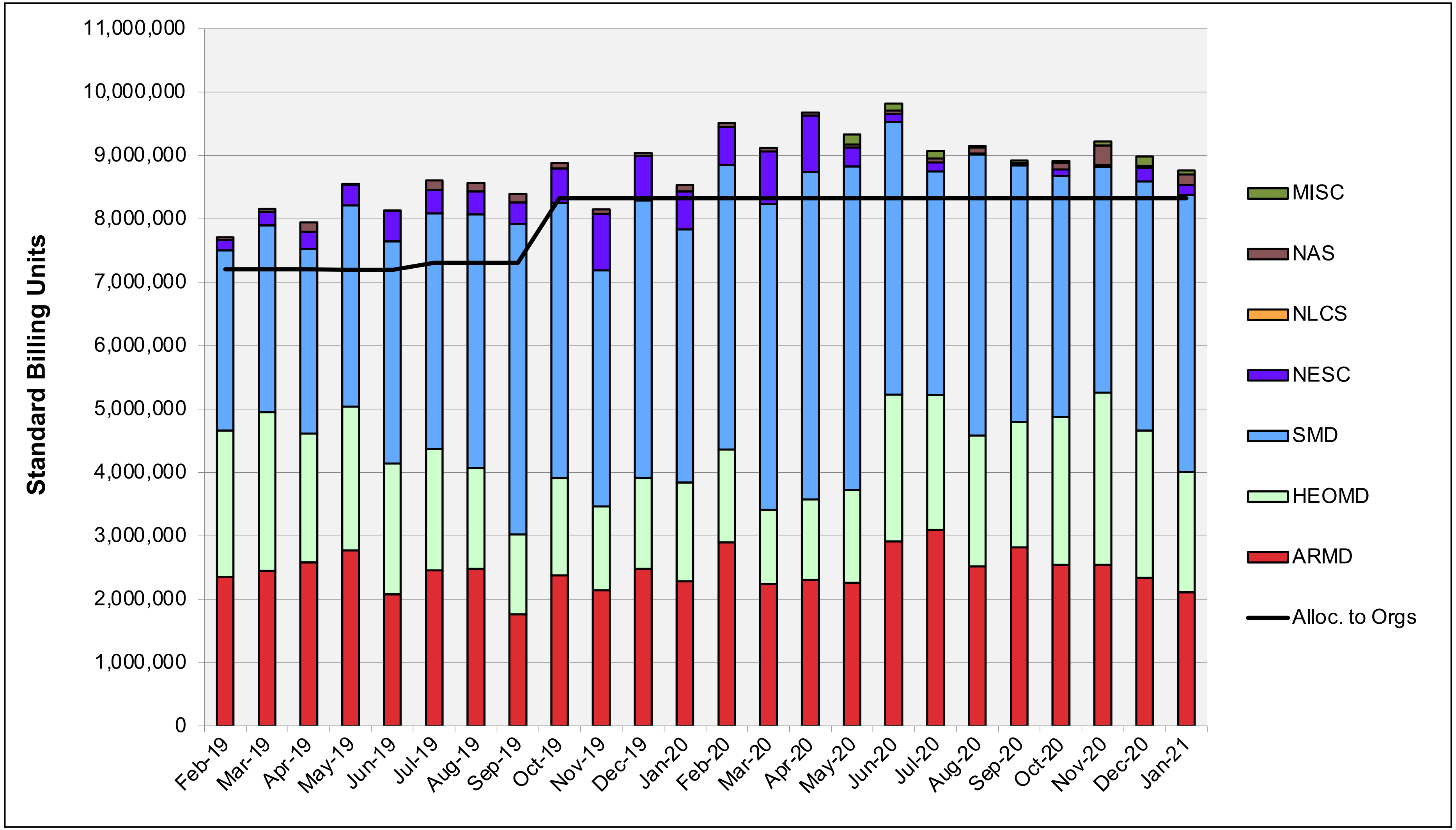
News and Events: Social Media

- **Coverage of NAS Stories**
  - Aeronautics Visualizations (Links back to SC20):
    - NASA Supercomputing: Facebook 547 users reached, 53 engagements, 20 likes, 7 shares; Twitter 1 retweet, 5 likes.
    - NAS: Twitter 2 retweets, 1 quote tweet, 7 likes.
  - NAS participation in NASA Day of Remembrance:
    - NAS: Twitter 1 retweet, 4 likes

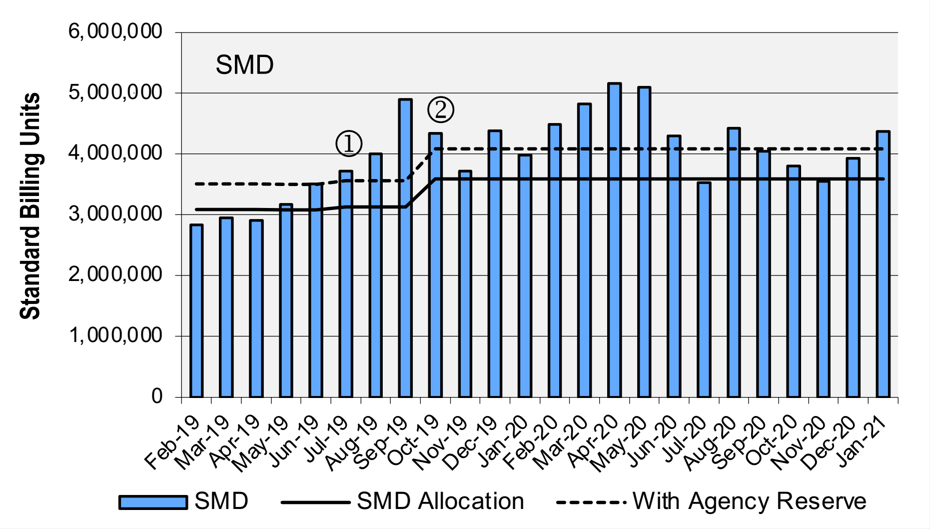
HECC Utilization

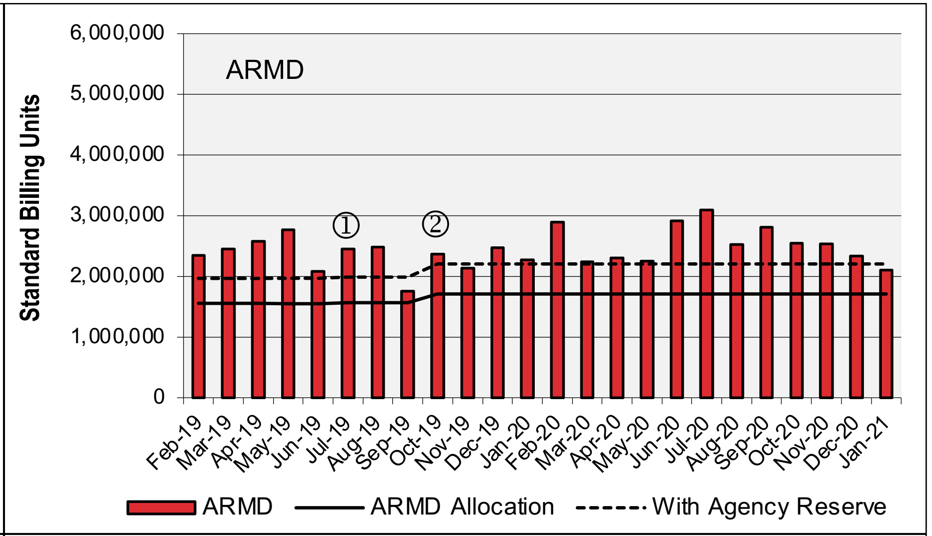


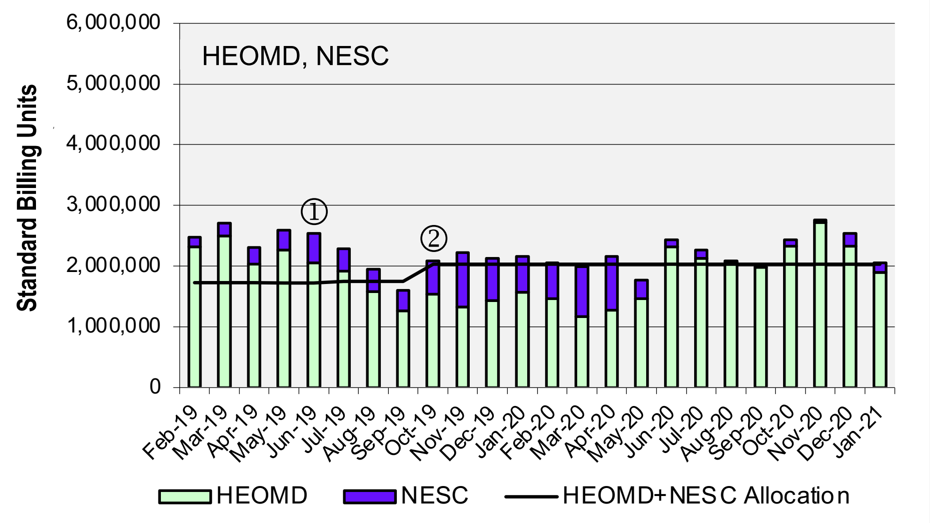
HECC Utilization Normalized to 30-Day Month



HECC Utilization Normalized to 30-Day Month



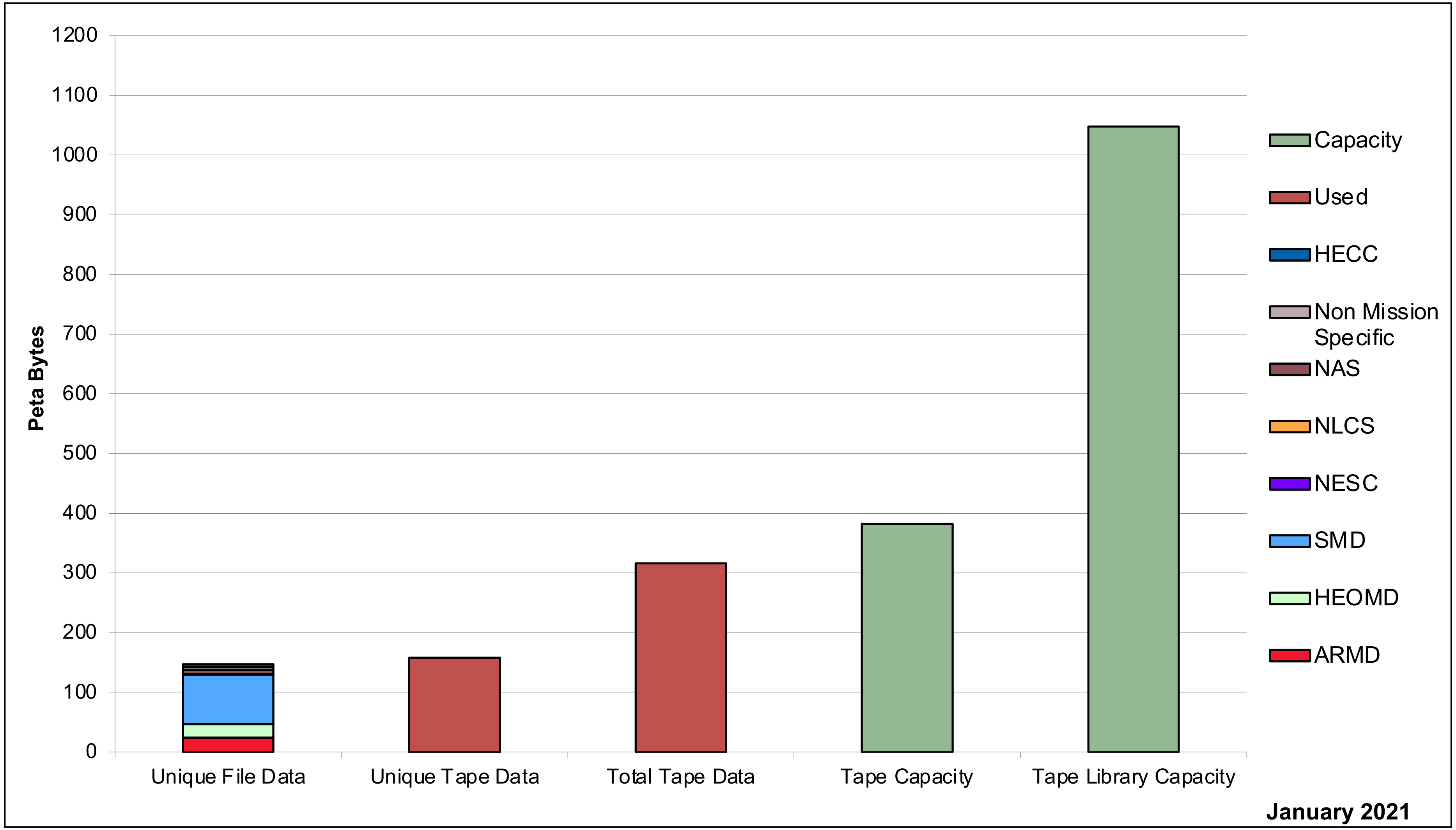




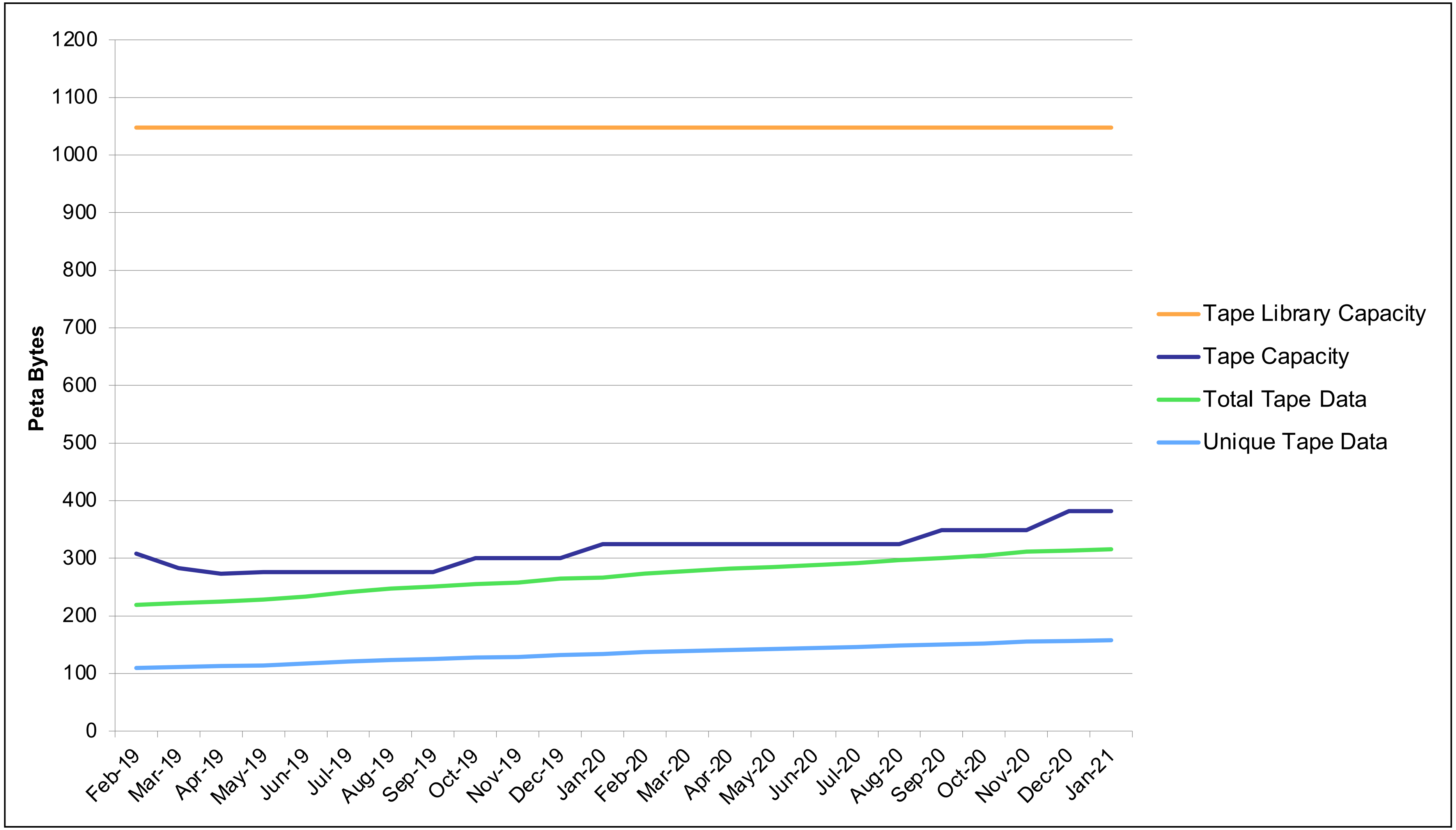
① Skylake Tesla GPU V100 Nodes installed

② 4 Cascade Lake E cells introduced into Aitken

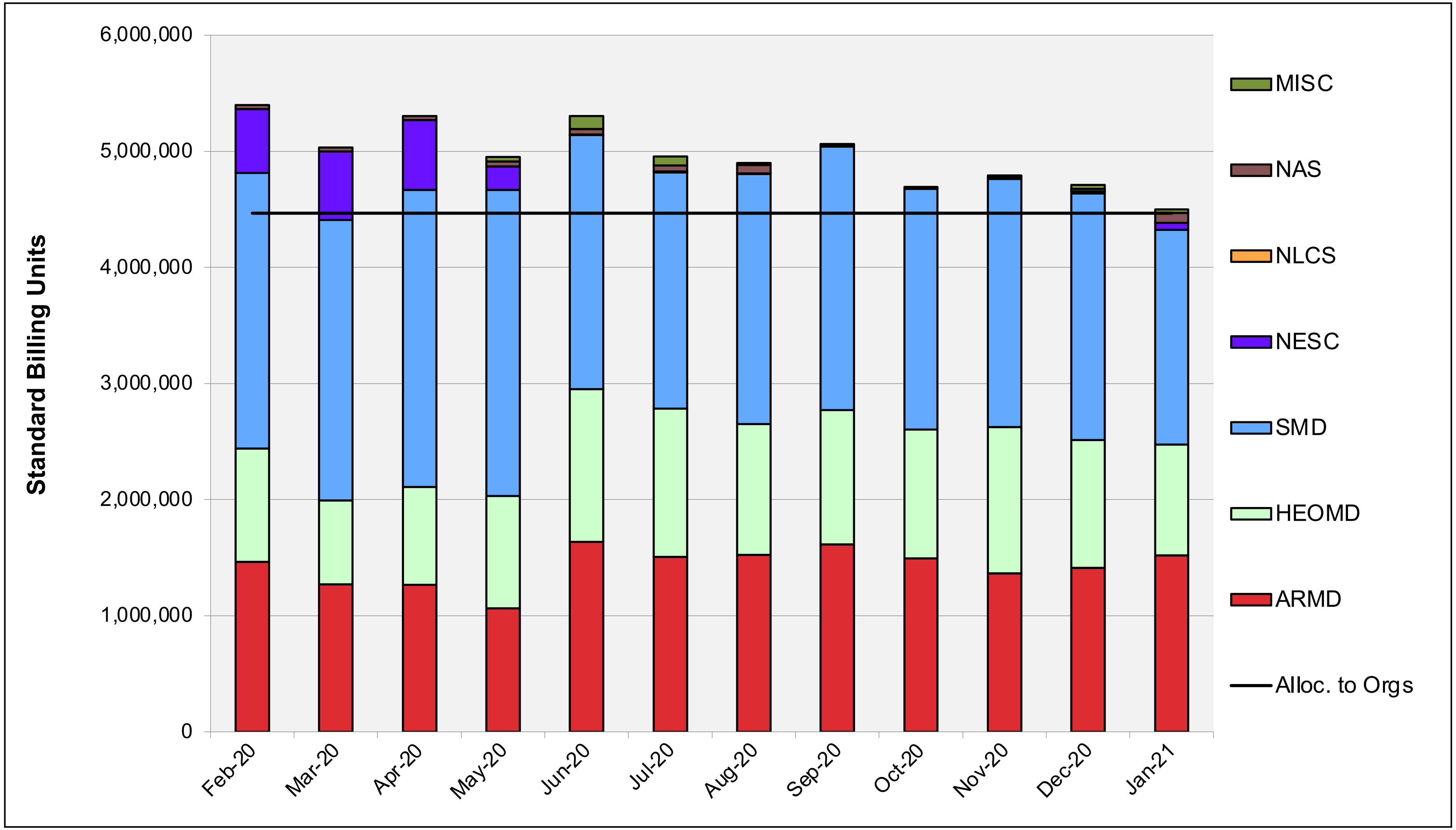
Tape Archive Status



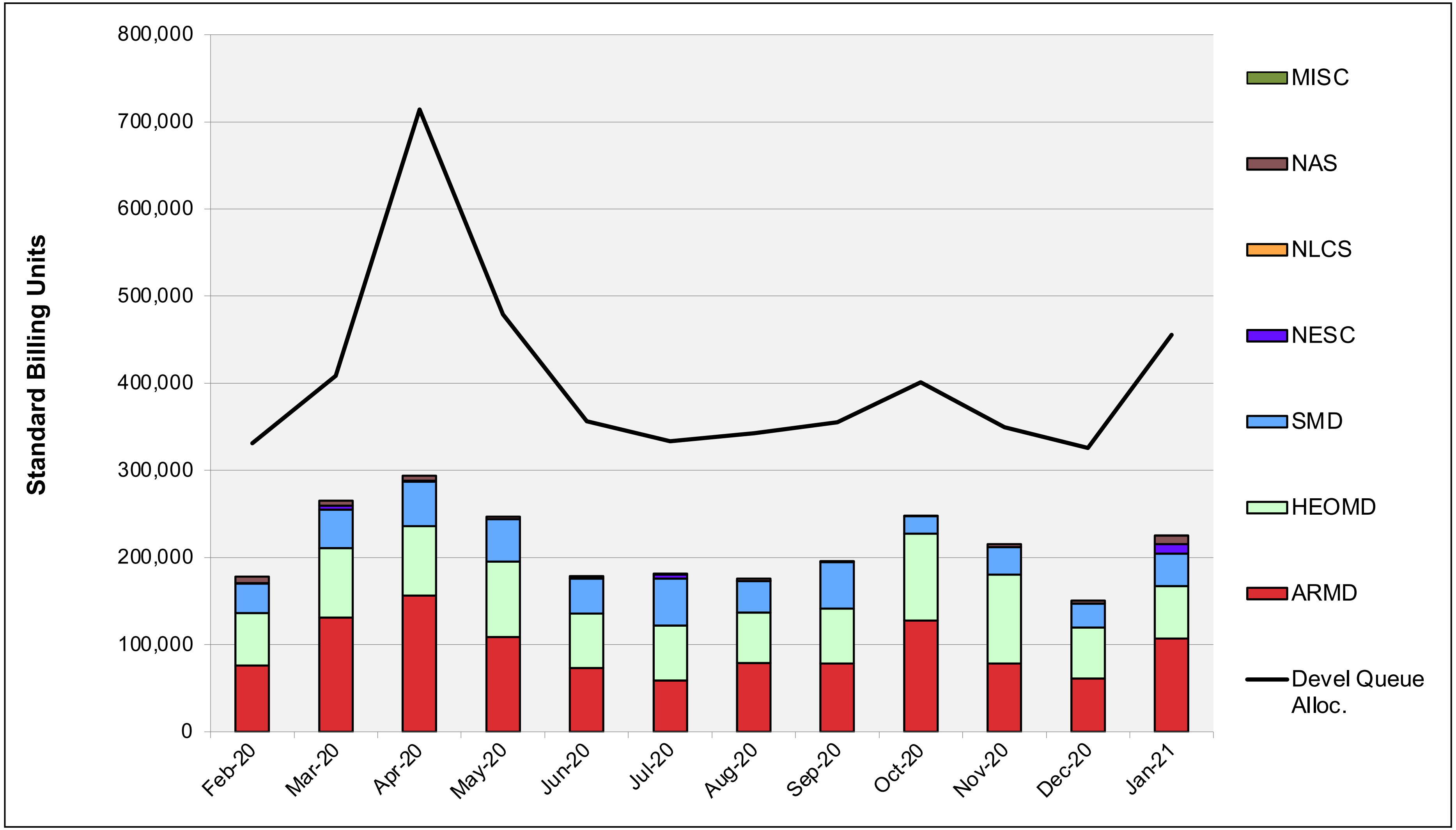
Tape Archive Status



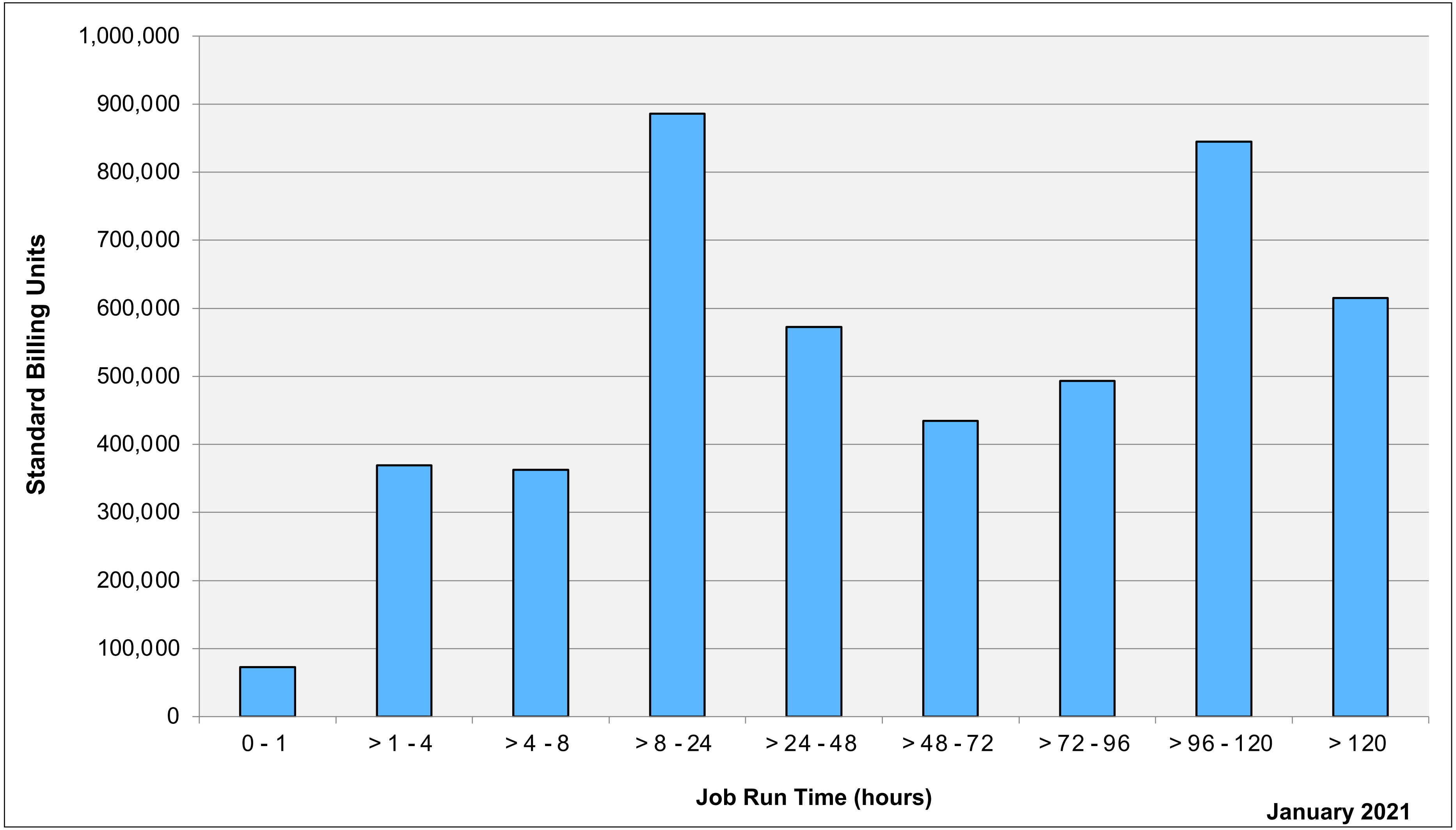
Pleiades: SBUs Reported, Normalized to 30-Day Month



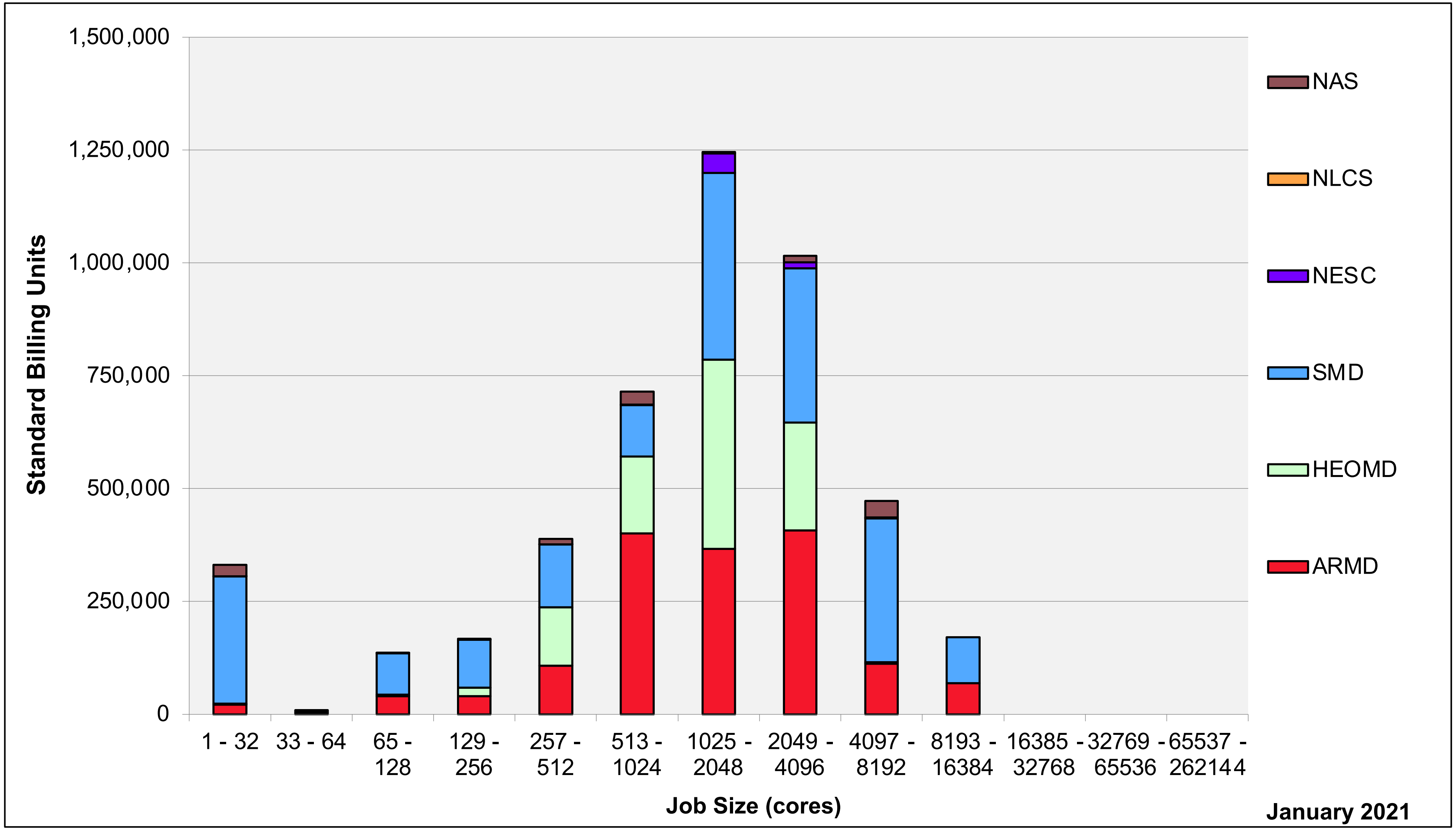
Pleiades: Devel Queue Utilization



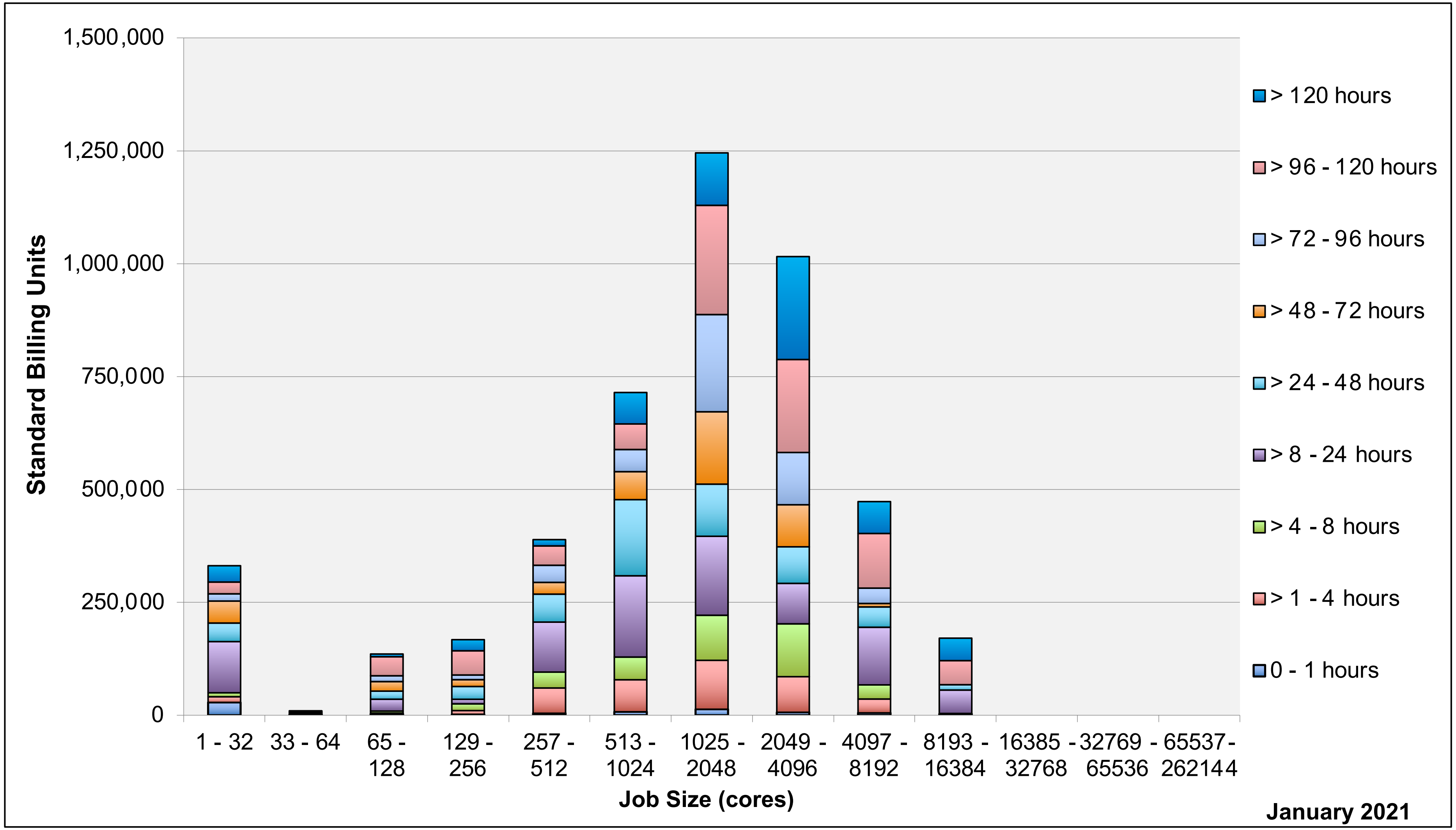
Pleiades: Monthly Utilization by Job Length



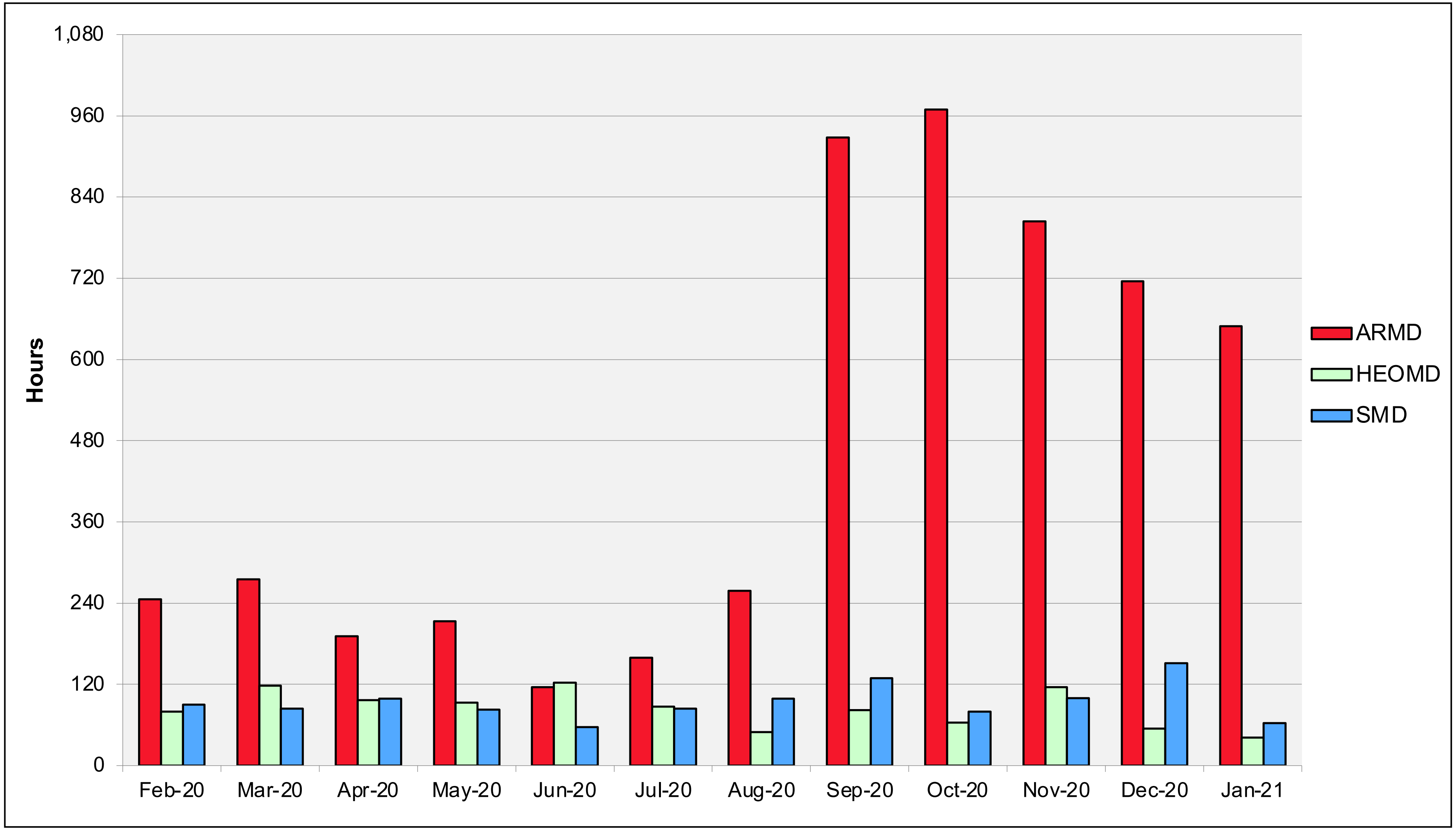
Pleiades: Monthly Utilization by Job Size



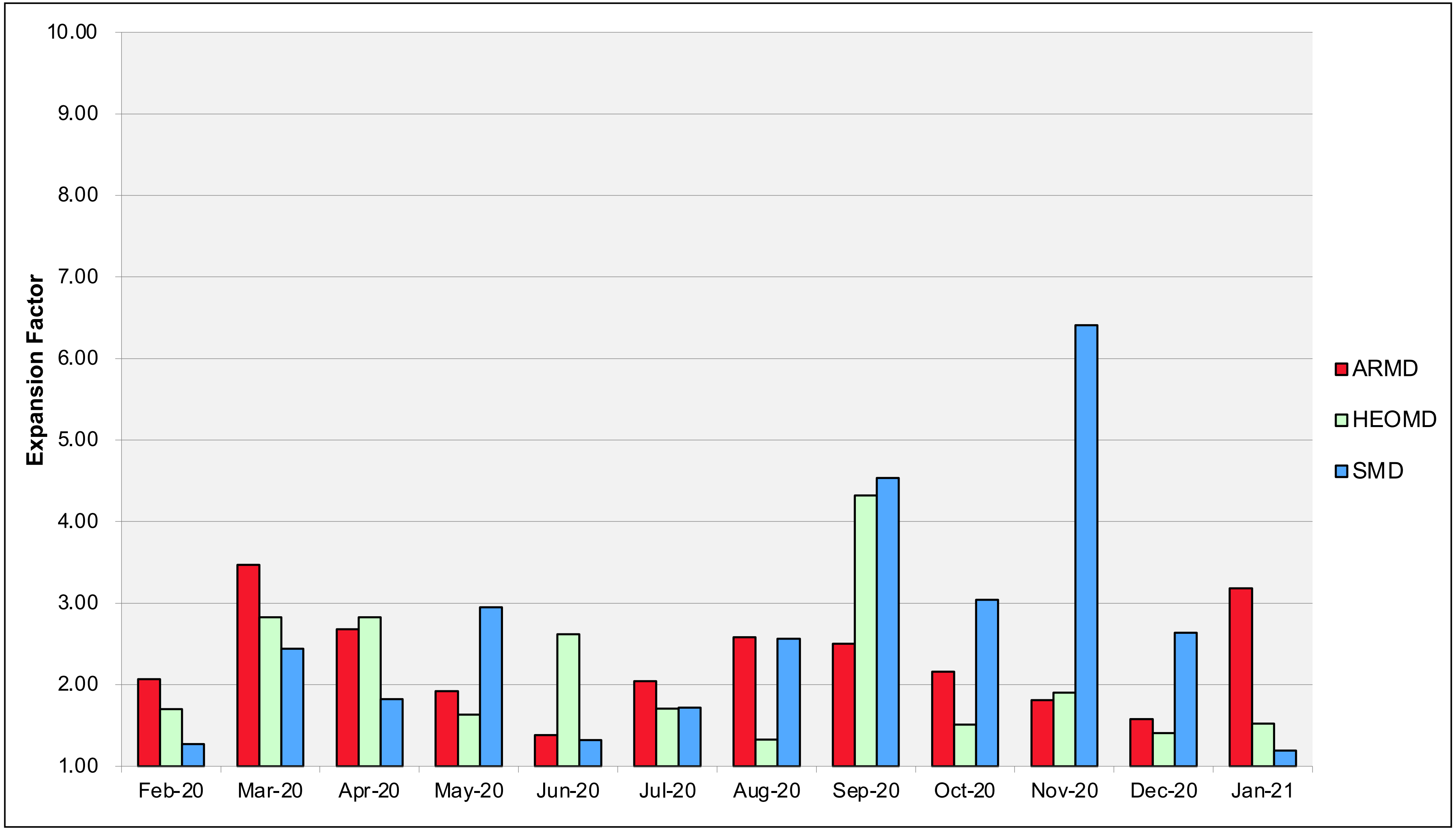
Pleiades: Monthly Utilization by Size and Length



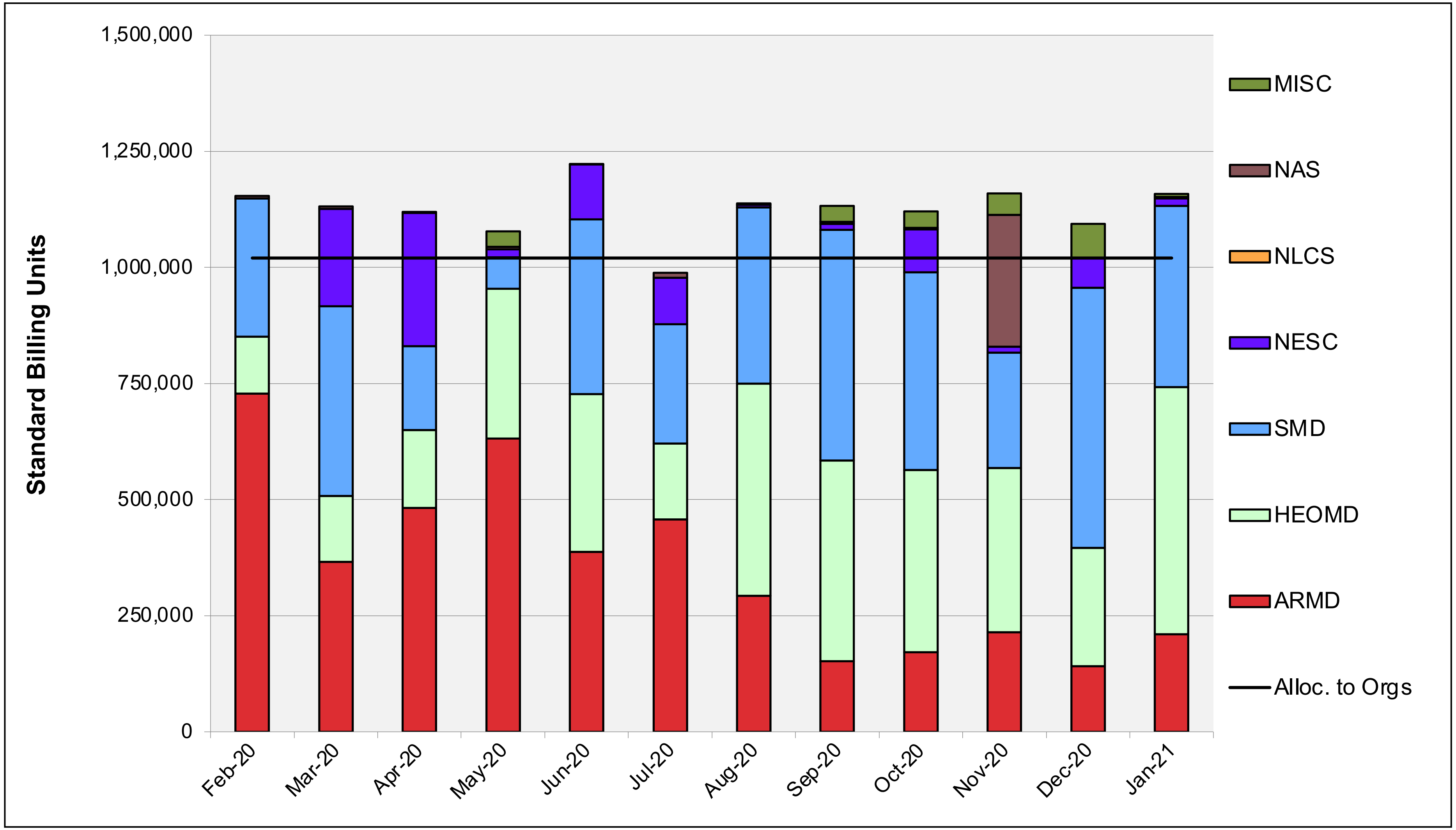
Pleiades: Average Time to Clear All Jobs



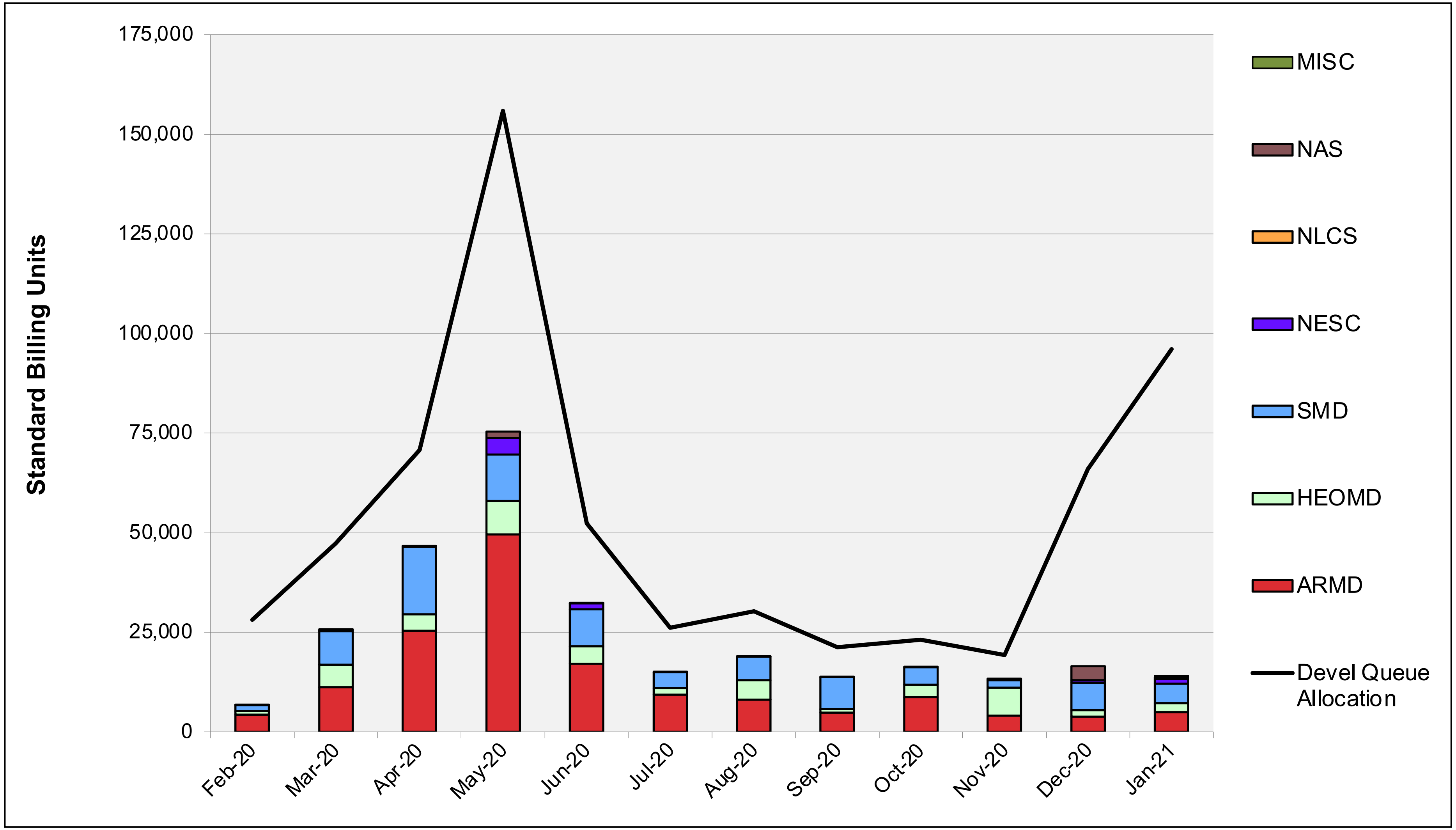
Pleiades: Average Expansion Factor



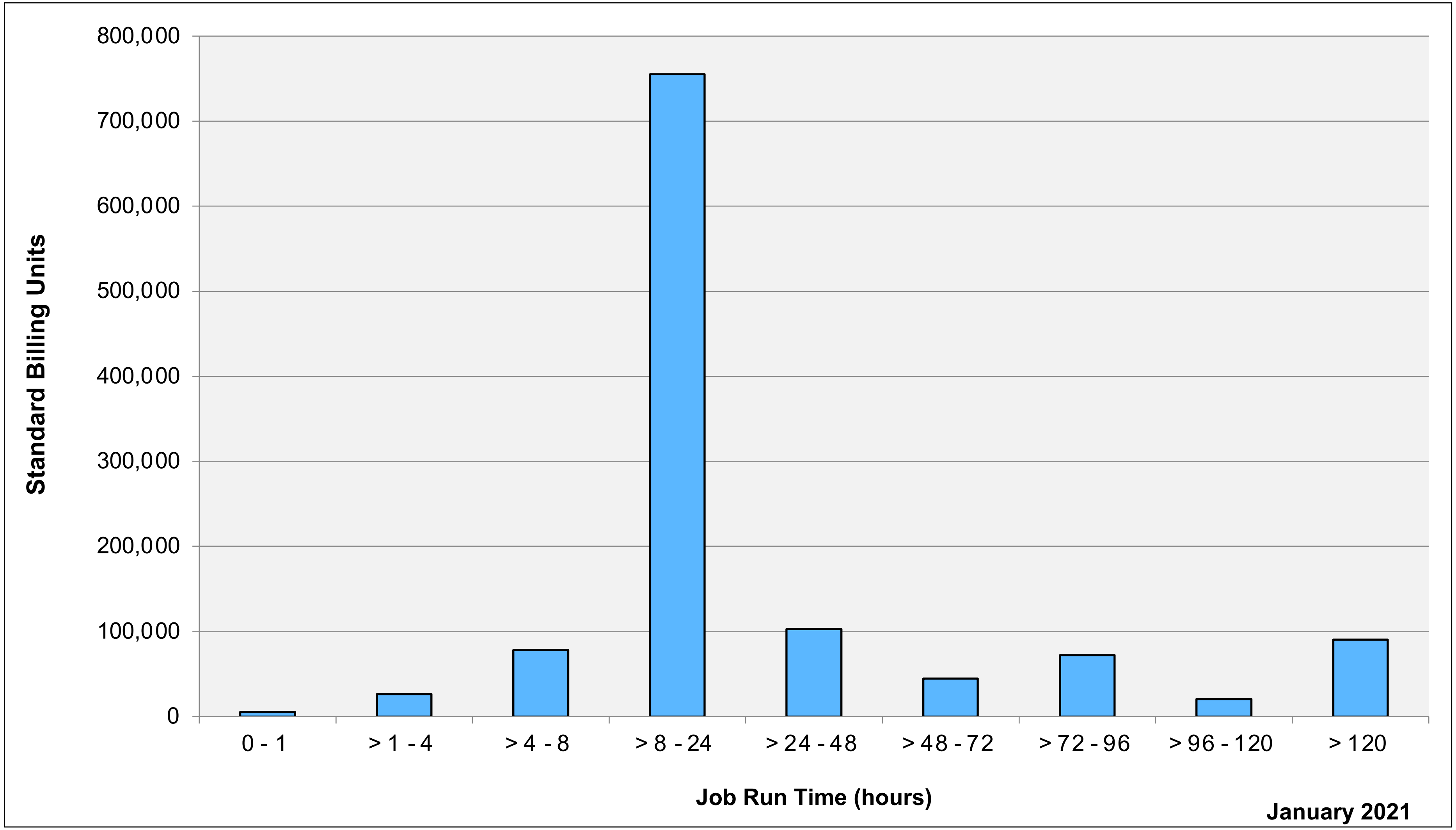
Aitken: SBUs Reported, Normalized to 30-Day Month



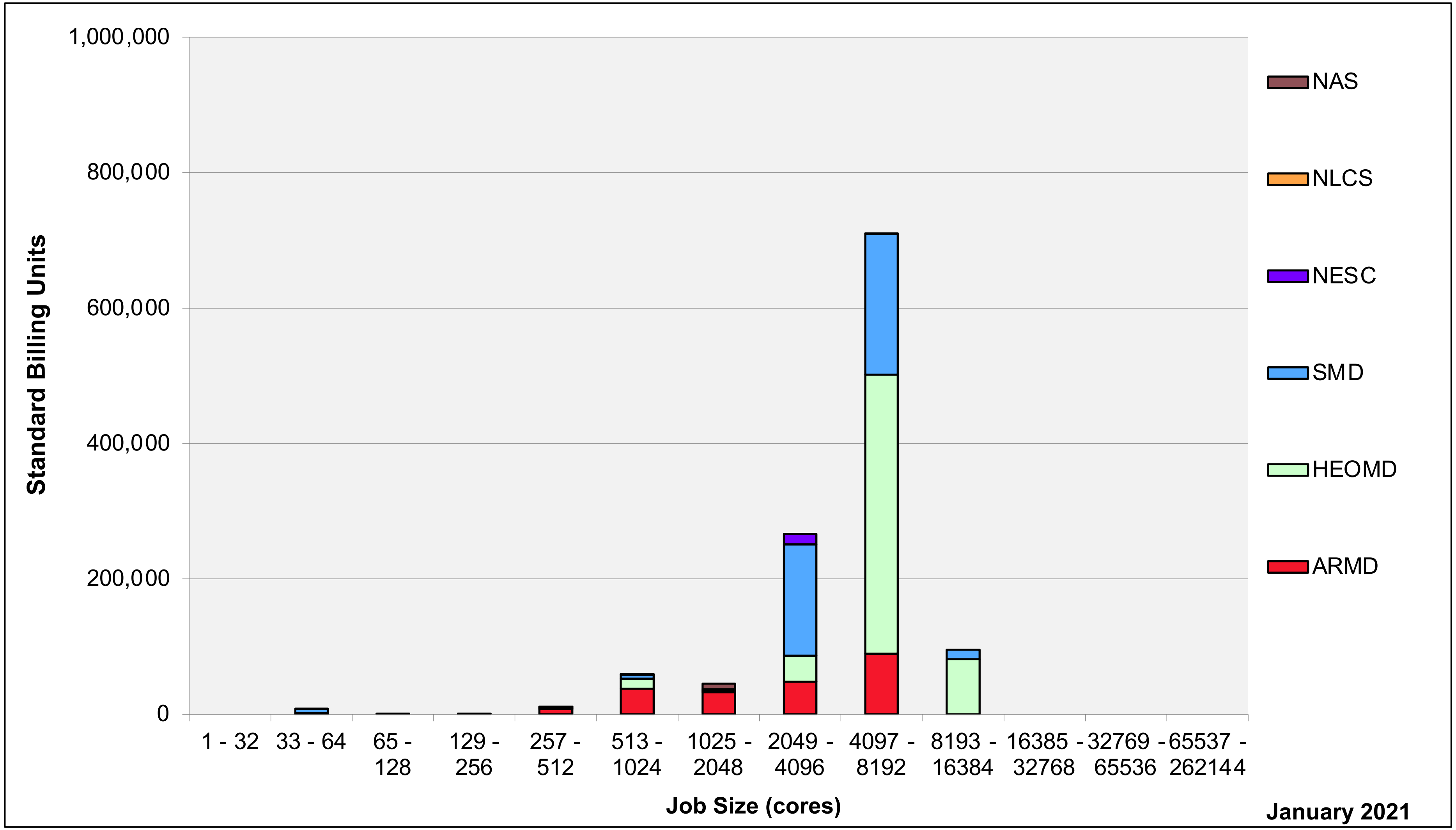
Aitken: Devel Queue Utilization



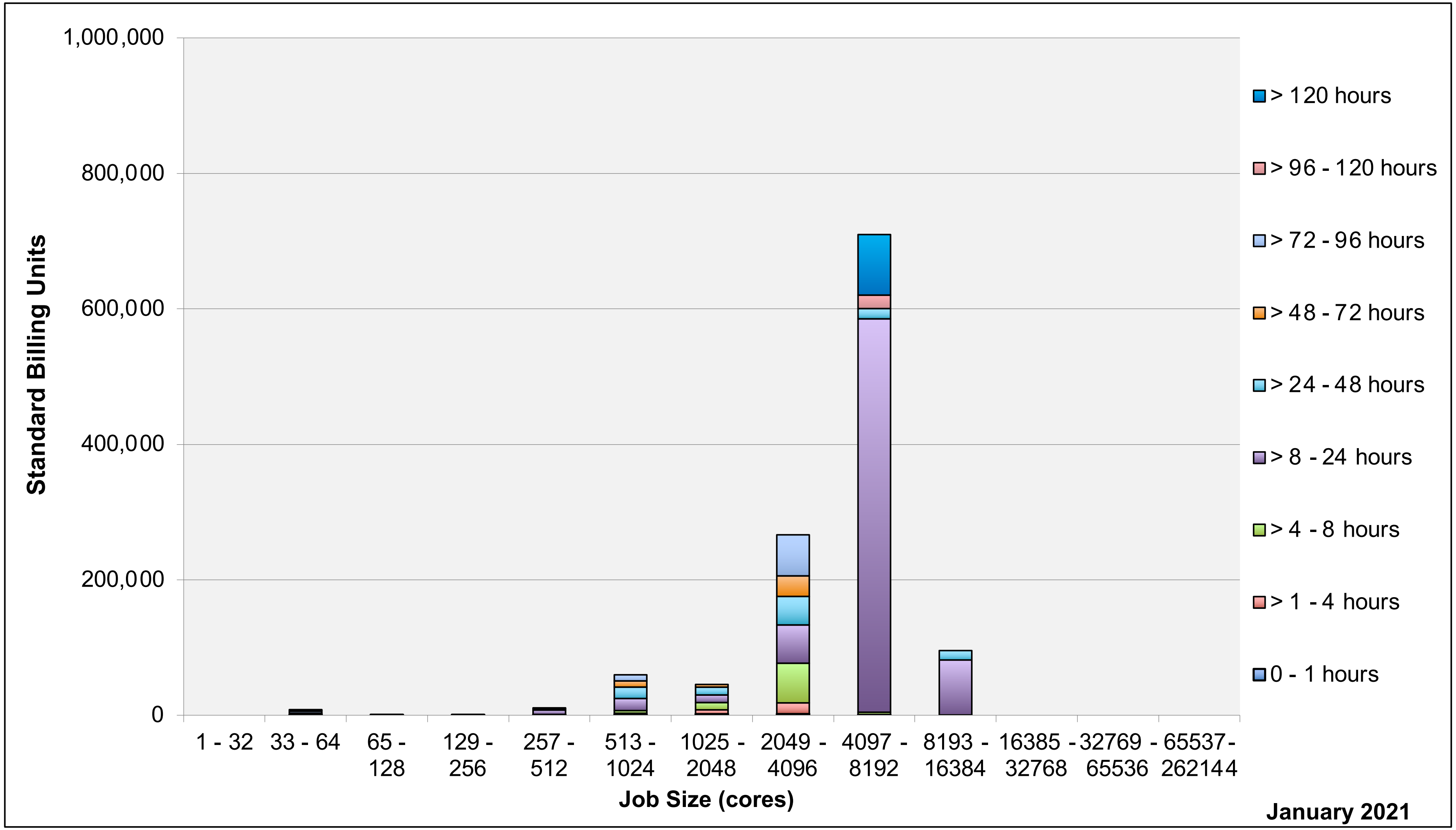
Aitken: Monthly Utilization by Job Length



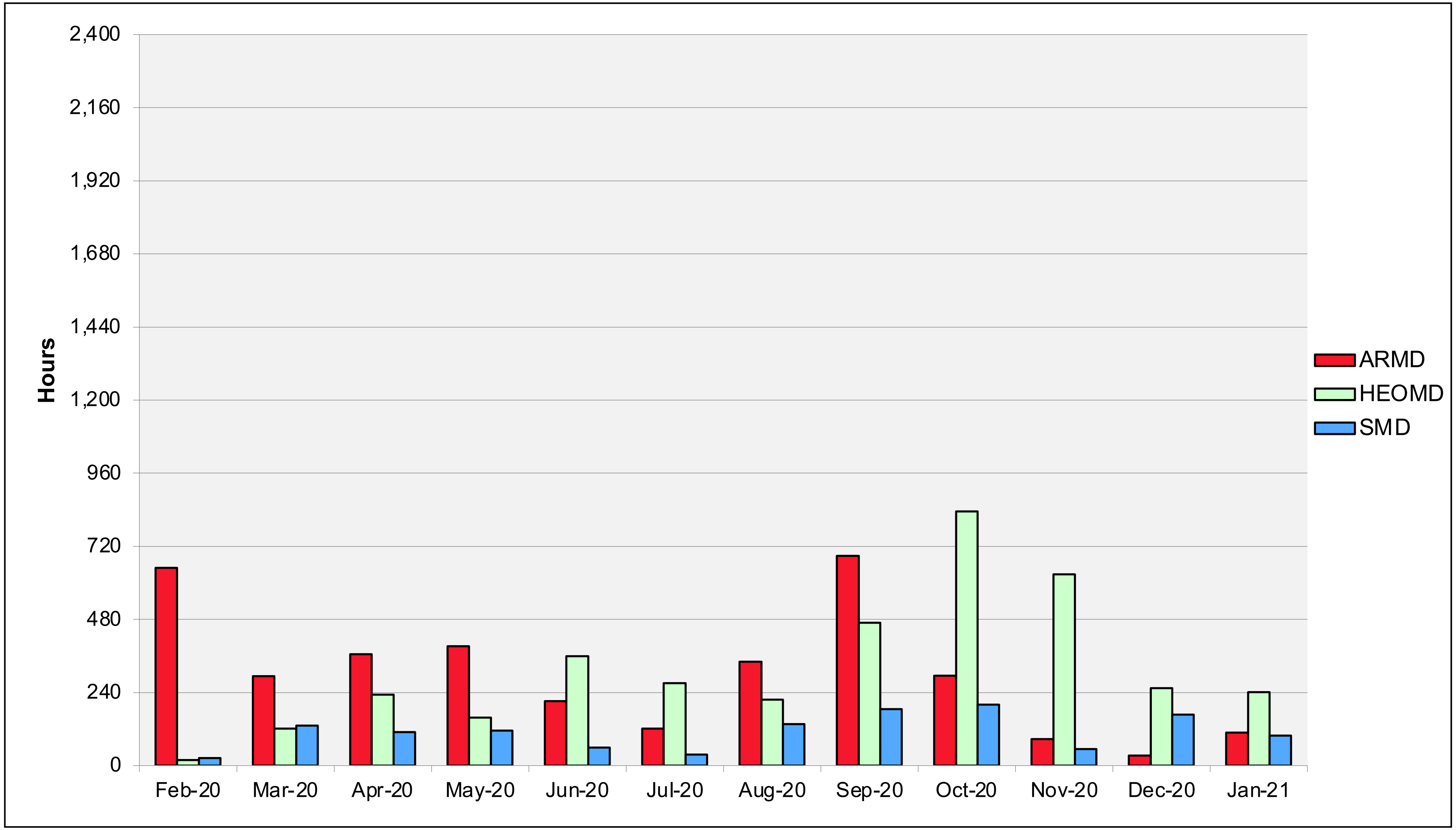
Aitken: Monthly Utilization by Job Size



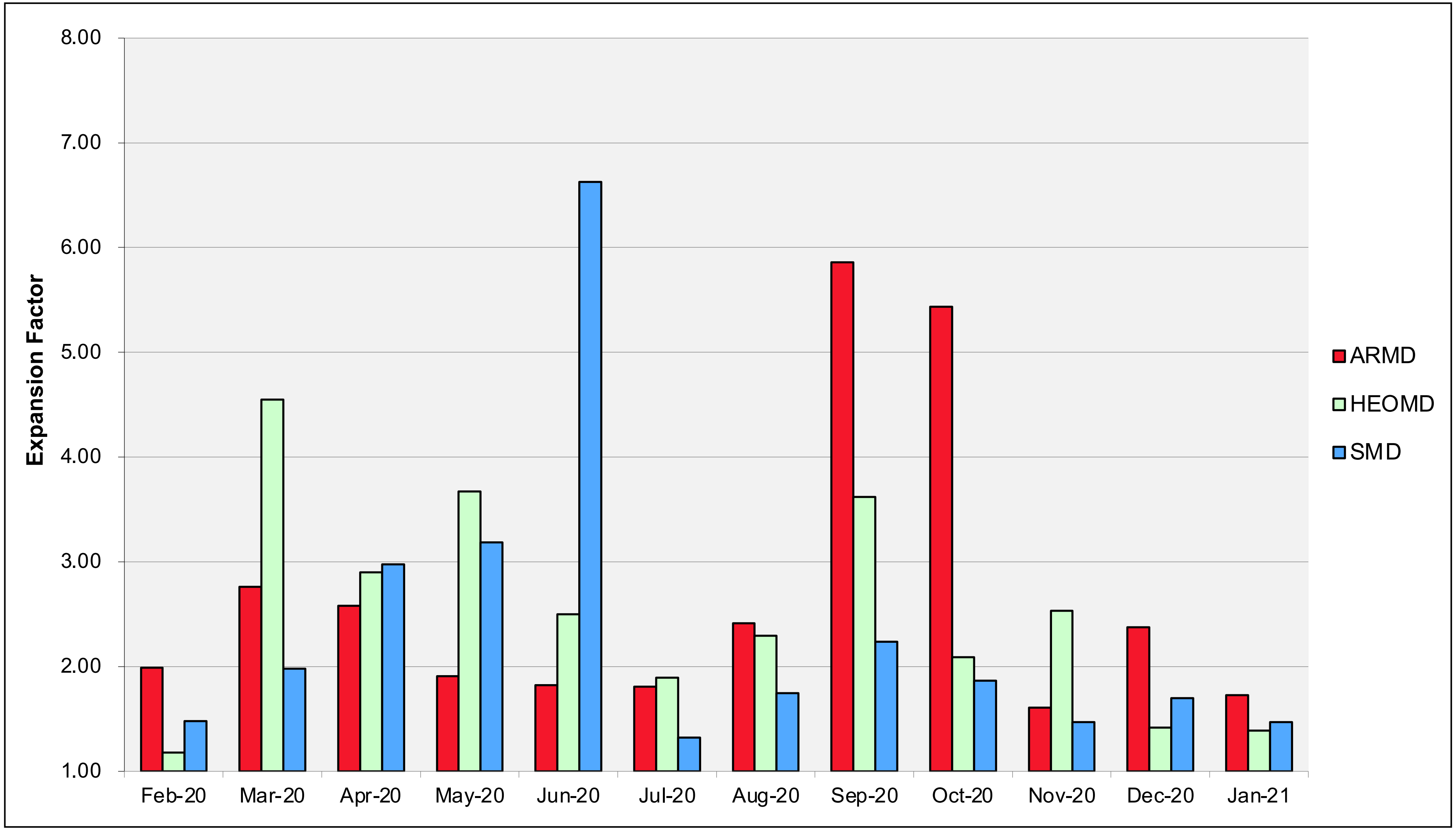
Aitken: Monthly Utilization by Size and Length



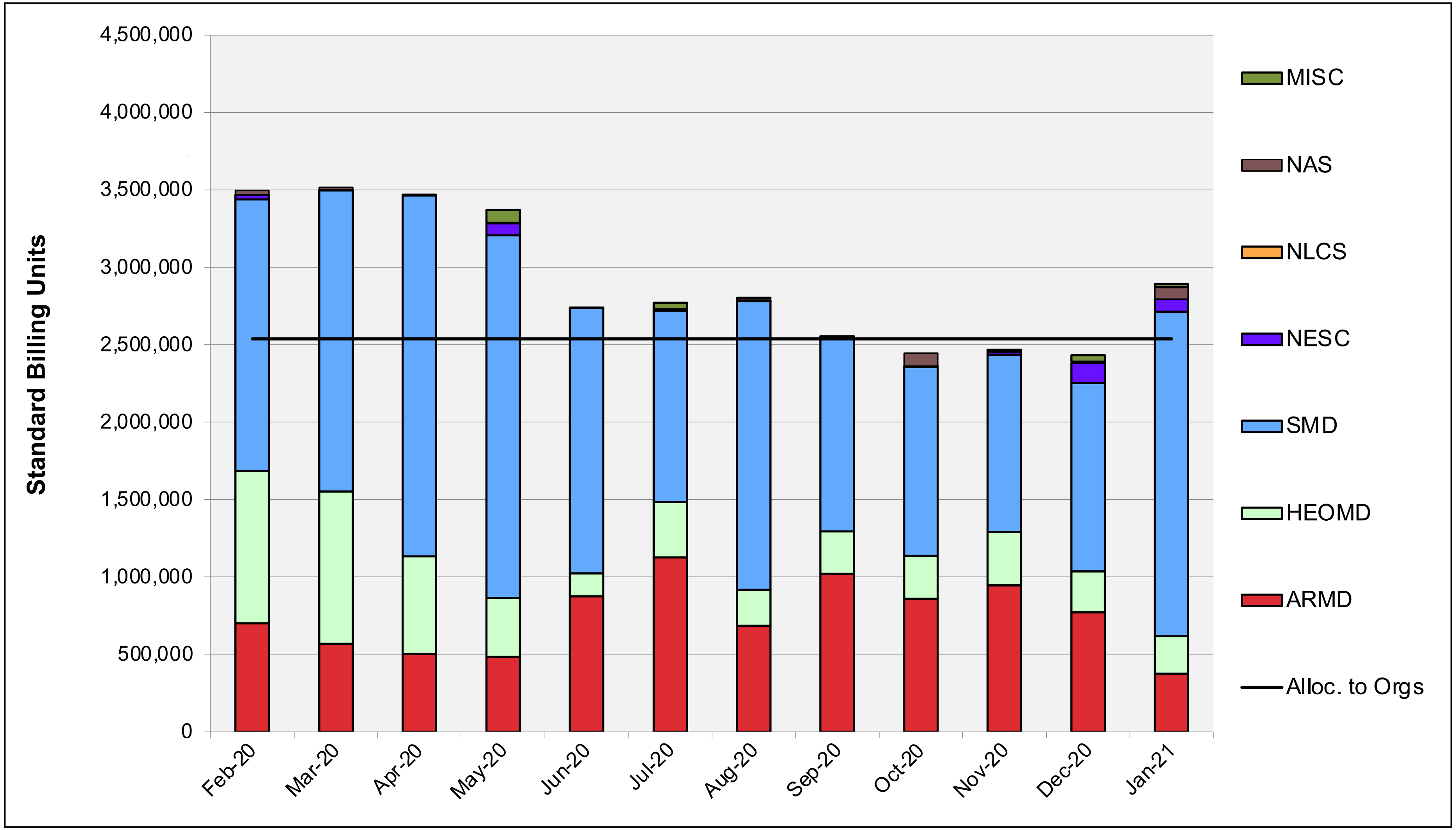
Aitken: Average Time to Clear All Jobs



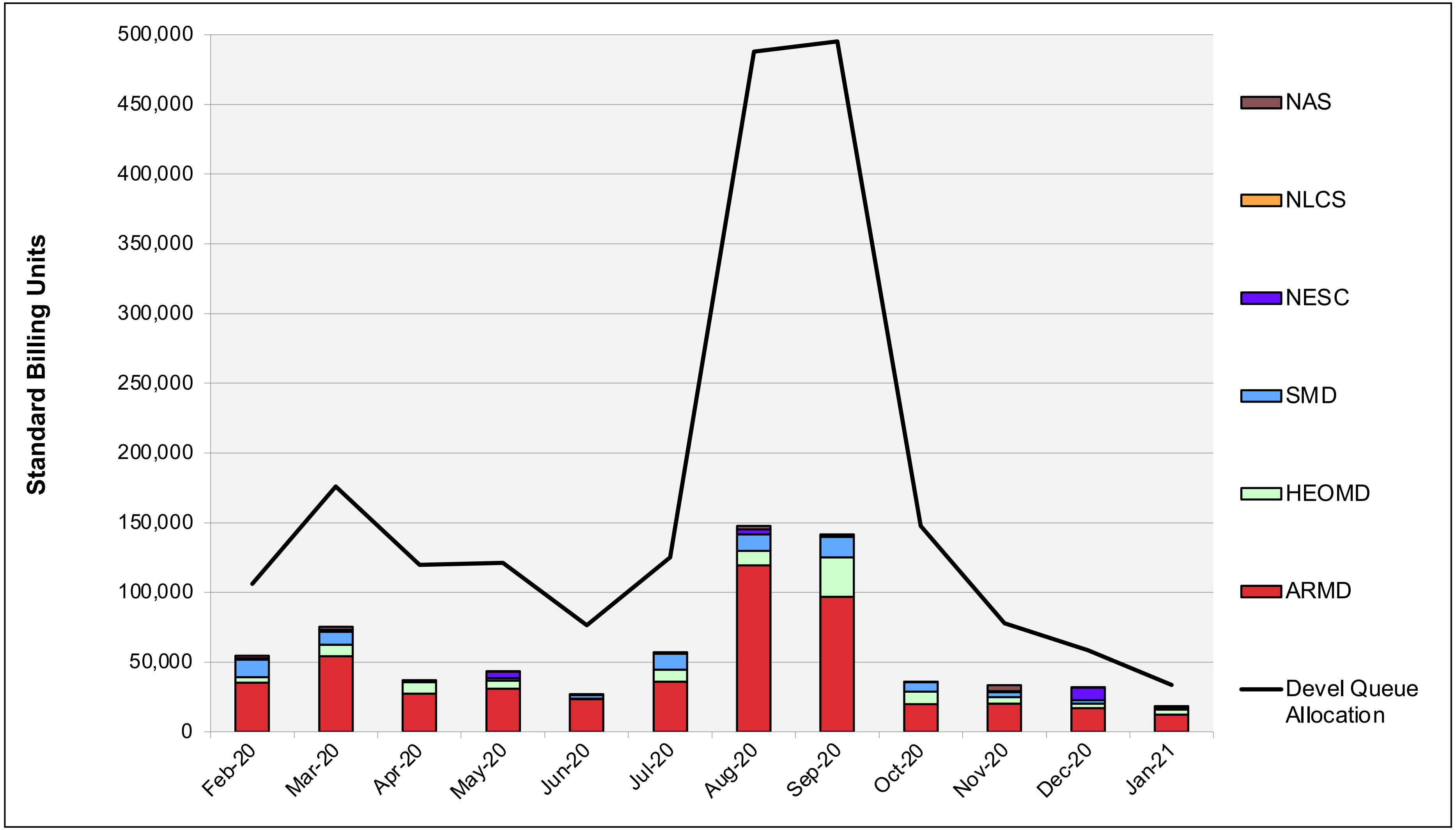
Aitken: Average Expansion Factor



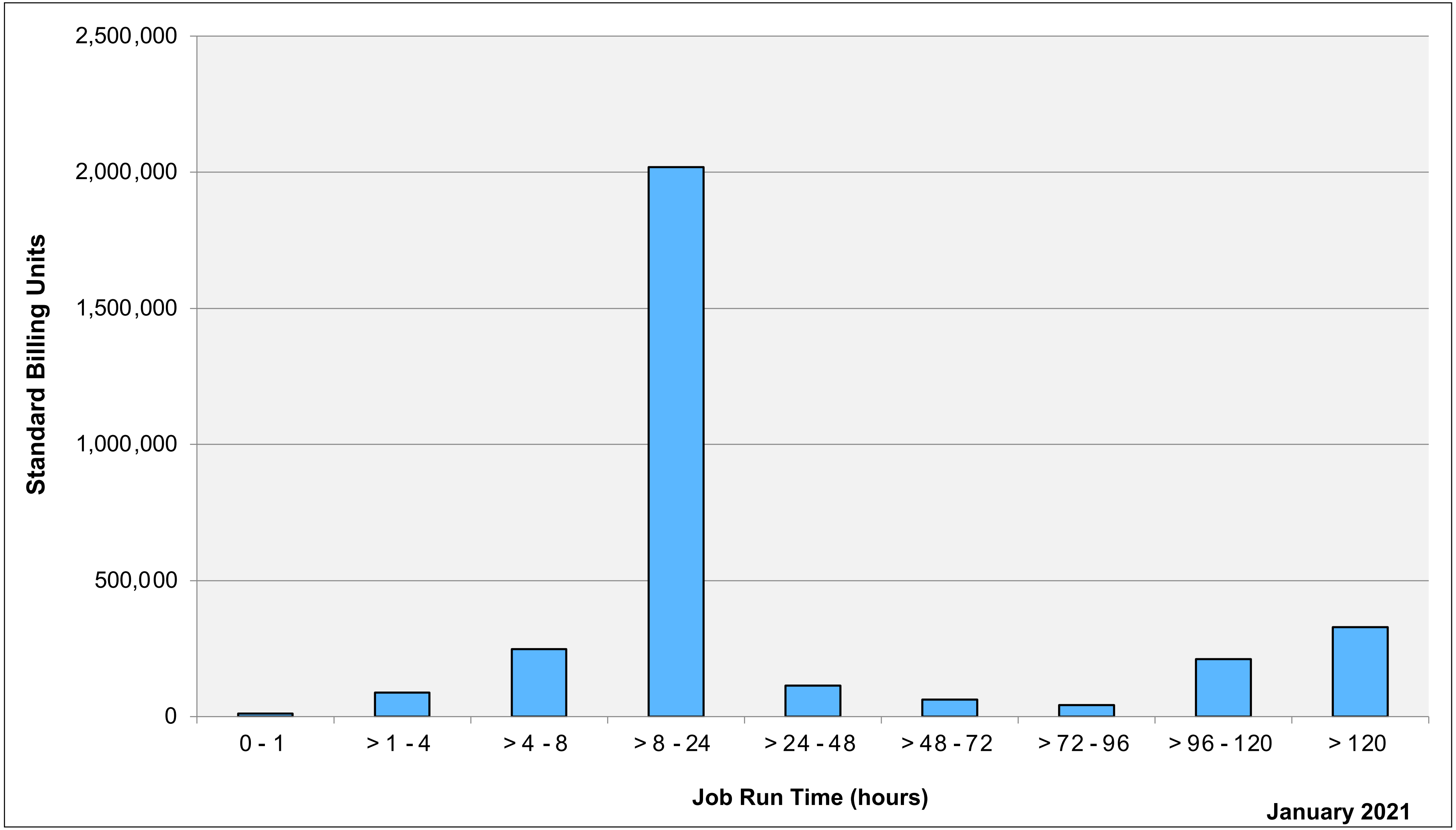
Electra: SBUs Reported, Normalized to 30-Day Month



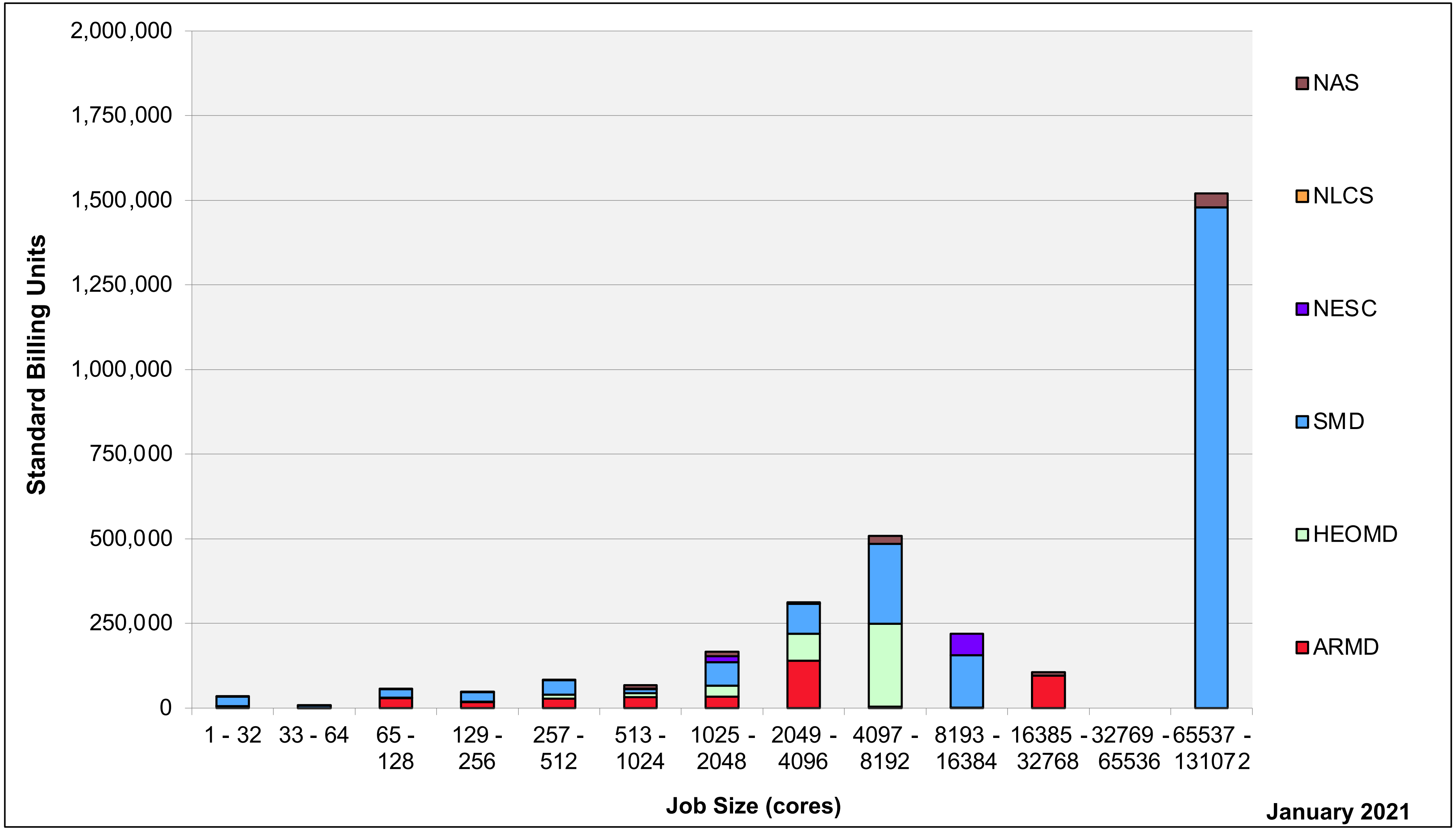
Electra: Devel Queue Utilization



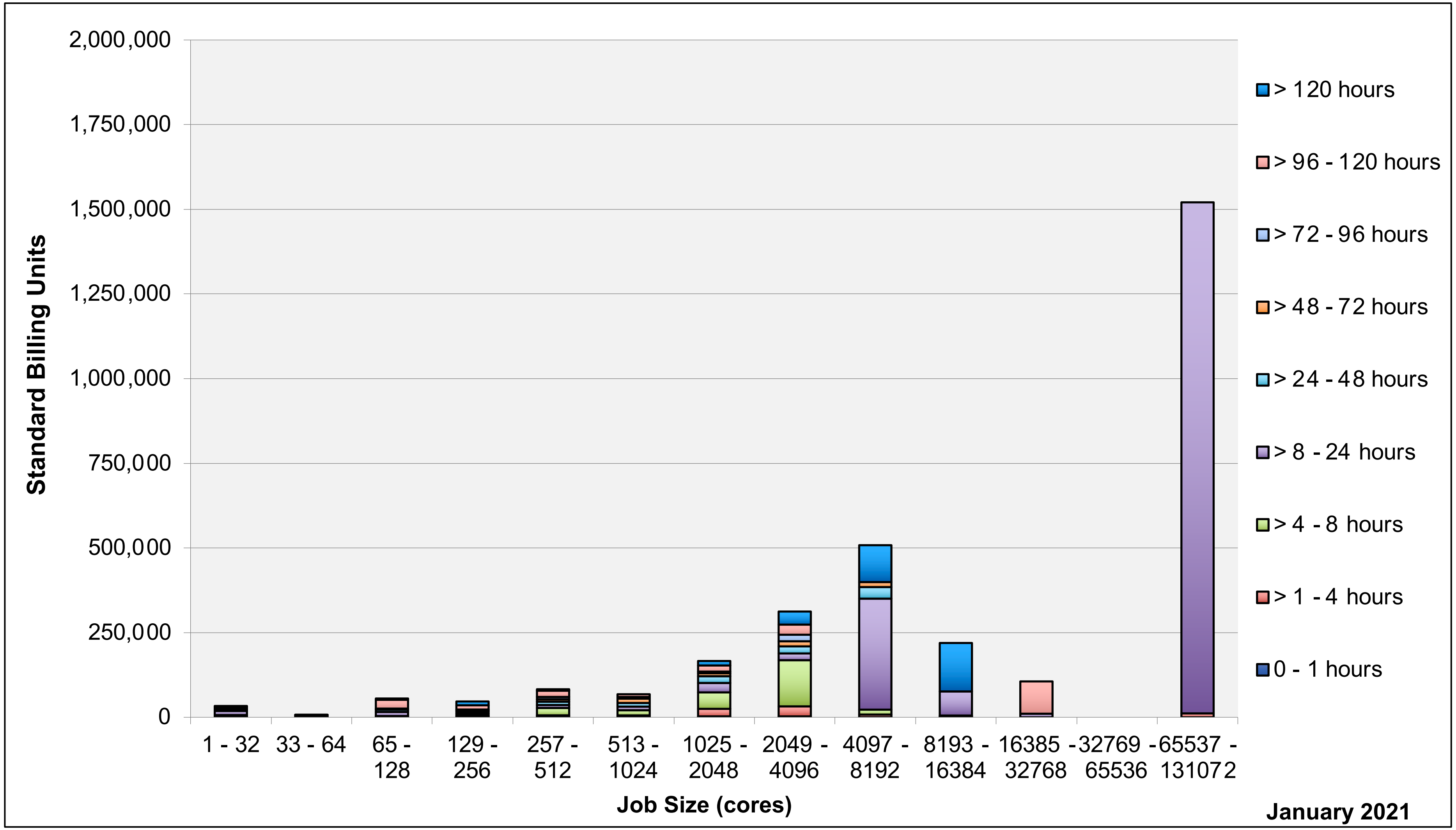
Electra: Monthly Utilization by Job Length



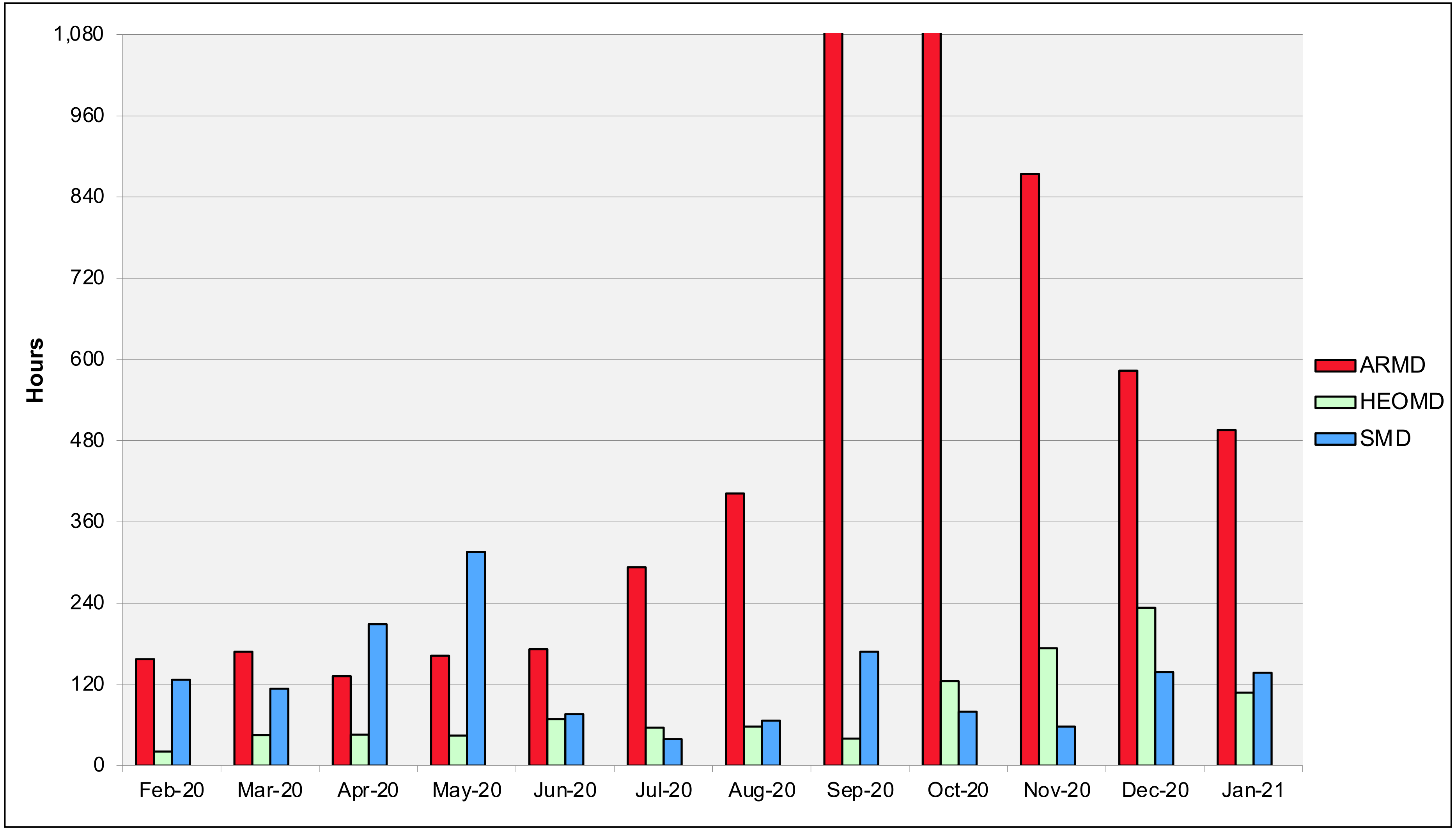
Electra: Monthly Utilization by Job Size



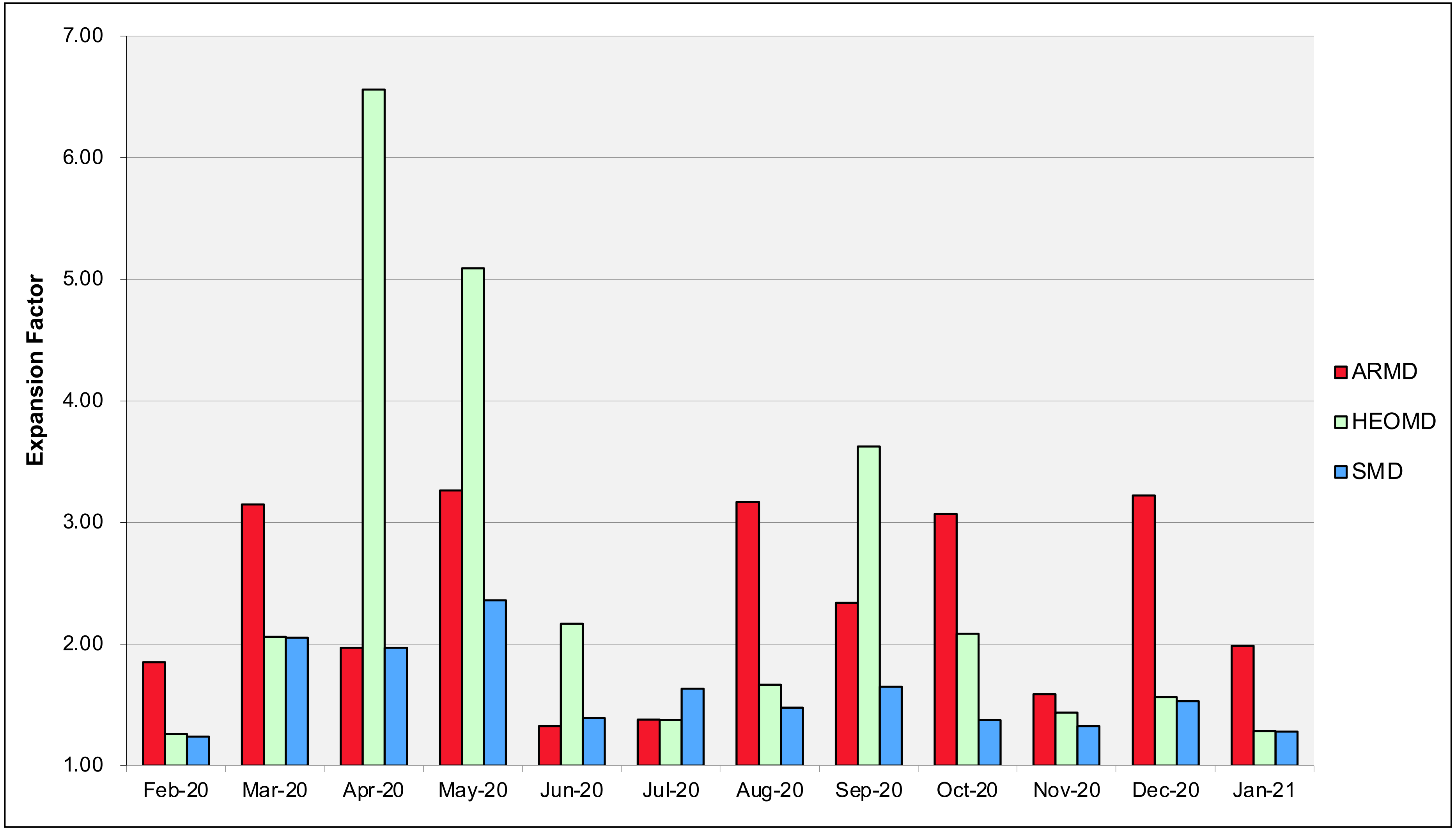
Electra: Monthly Utilization by Size and Length



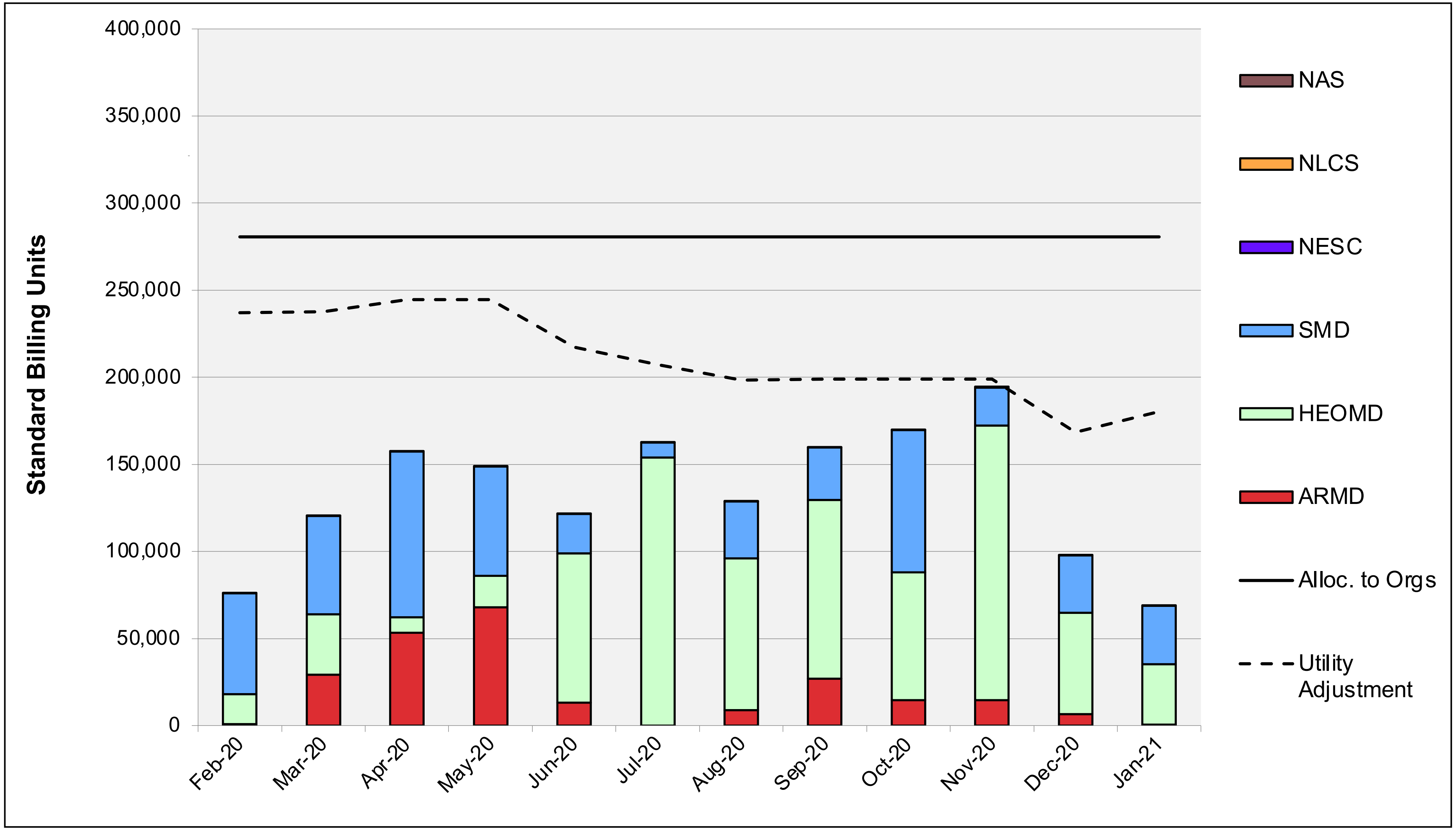
Electra: Average Time to Clear All Jobs



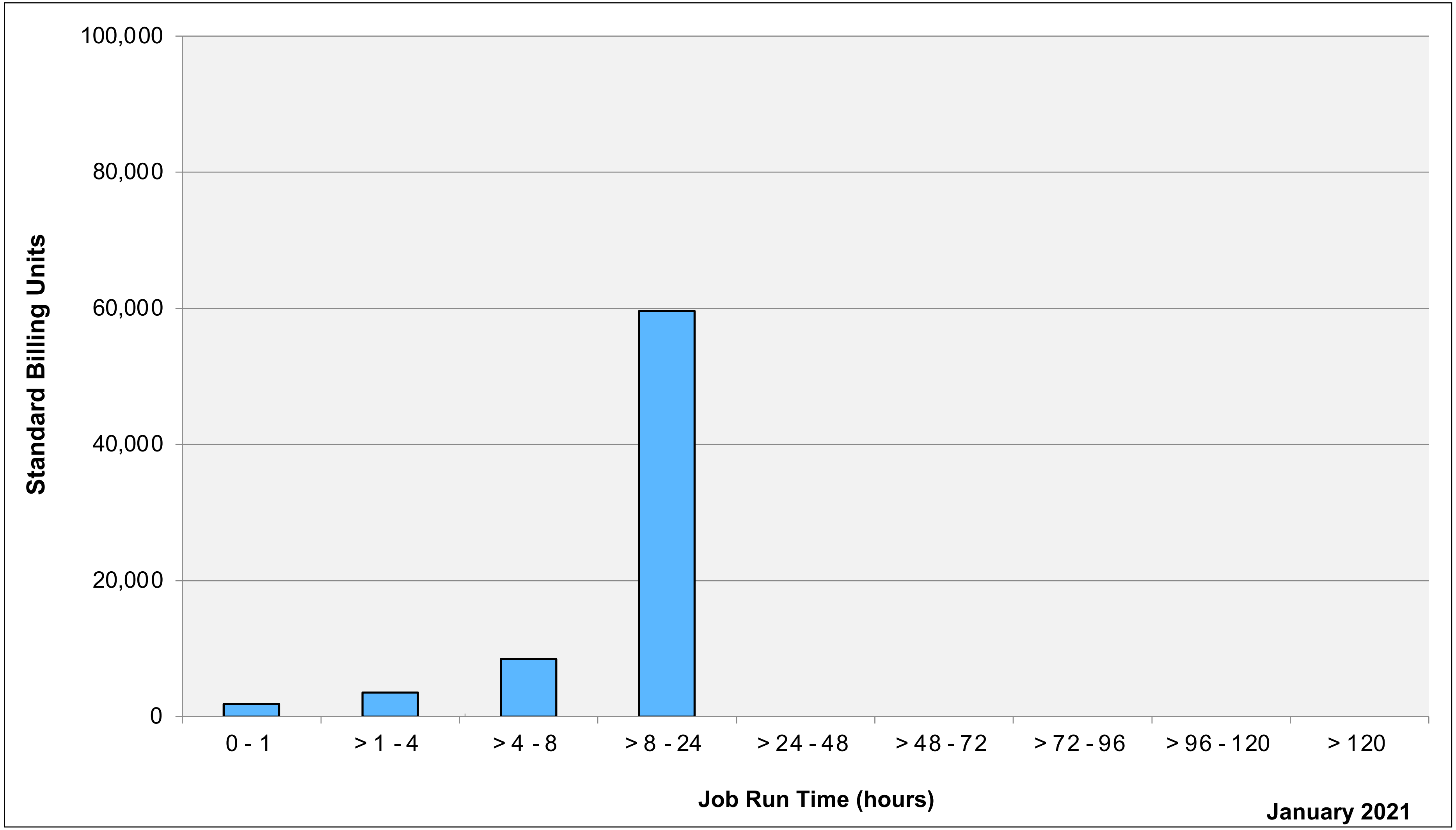
Electra: Average Expansion Factor



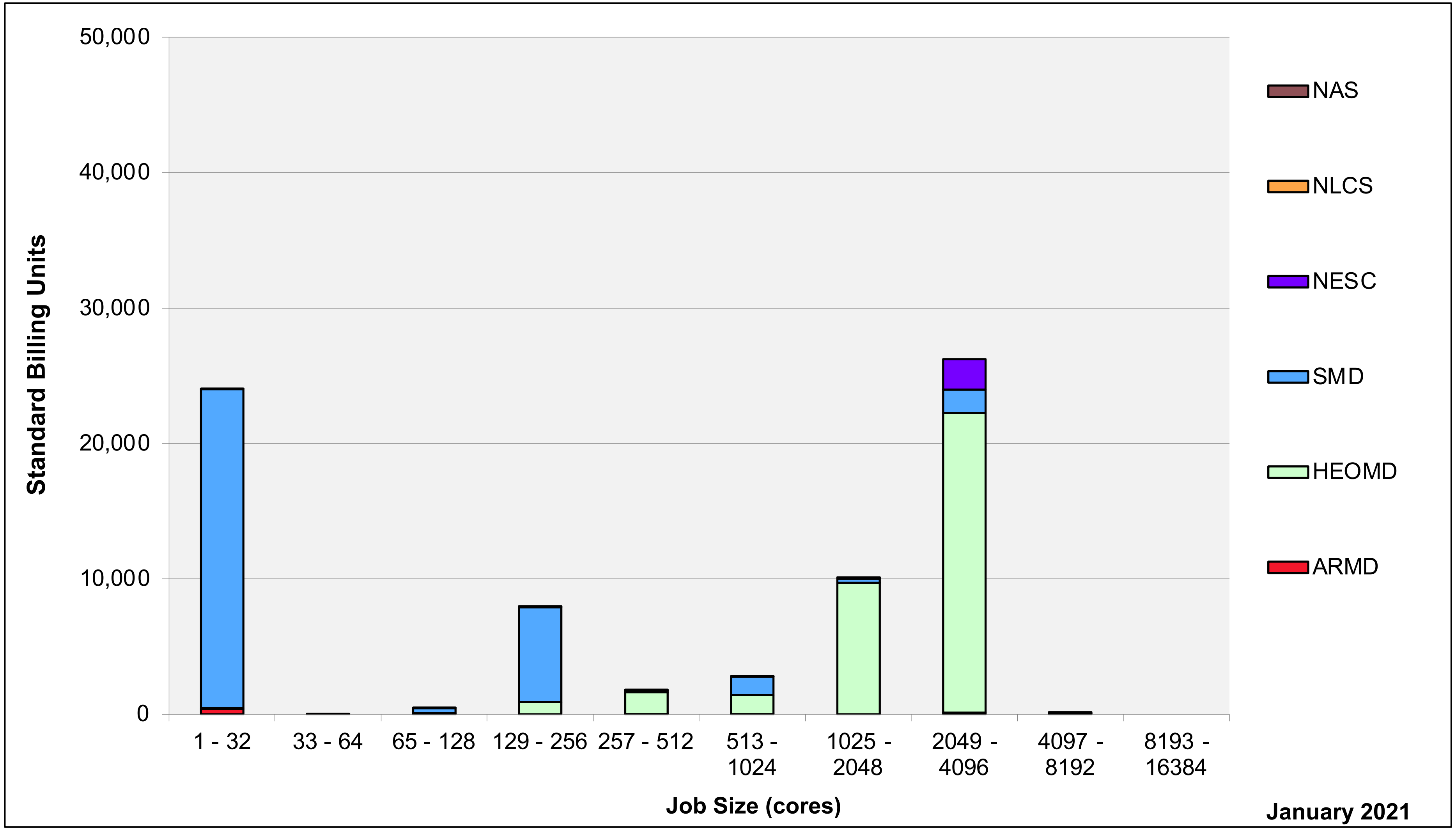
Merope: SBUs Reported, Normalized to 30-Day Month



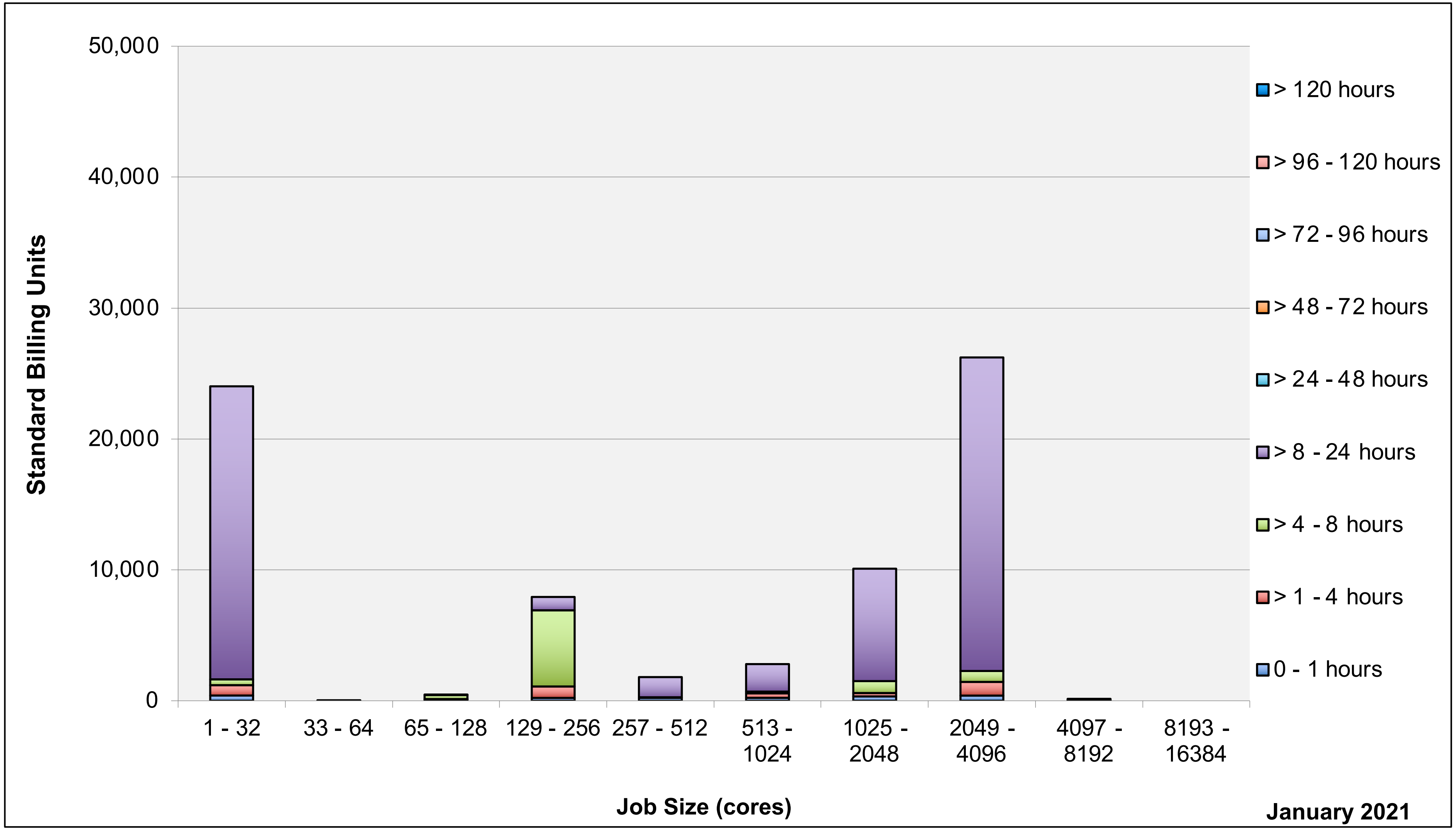
Merope: Monthly Utilization by Job Length



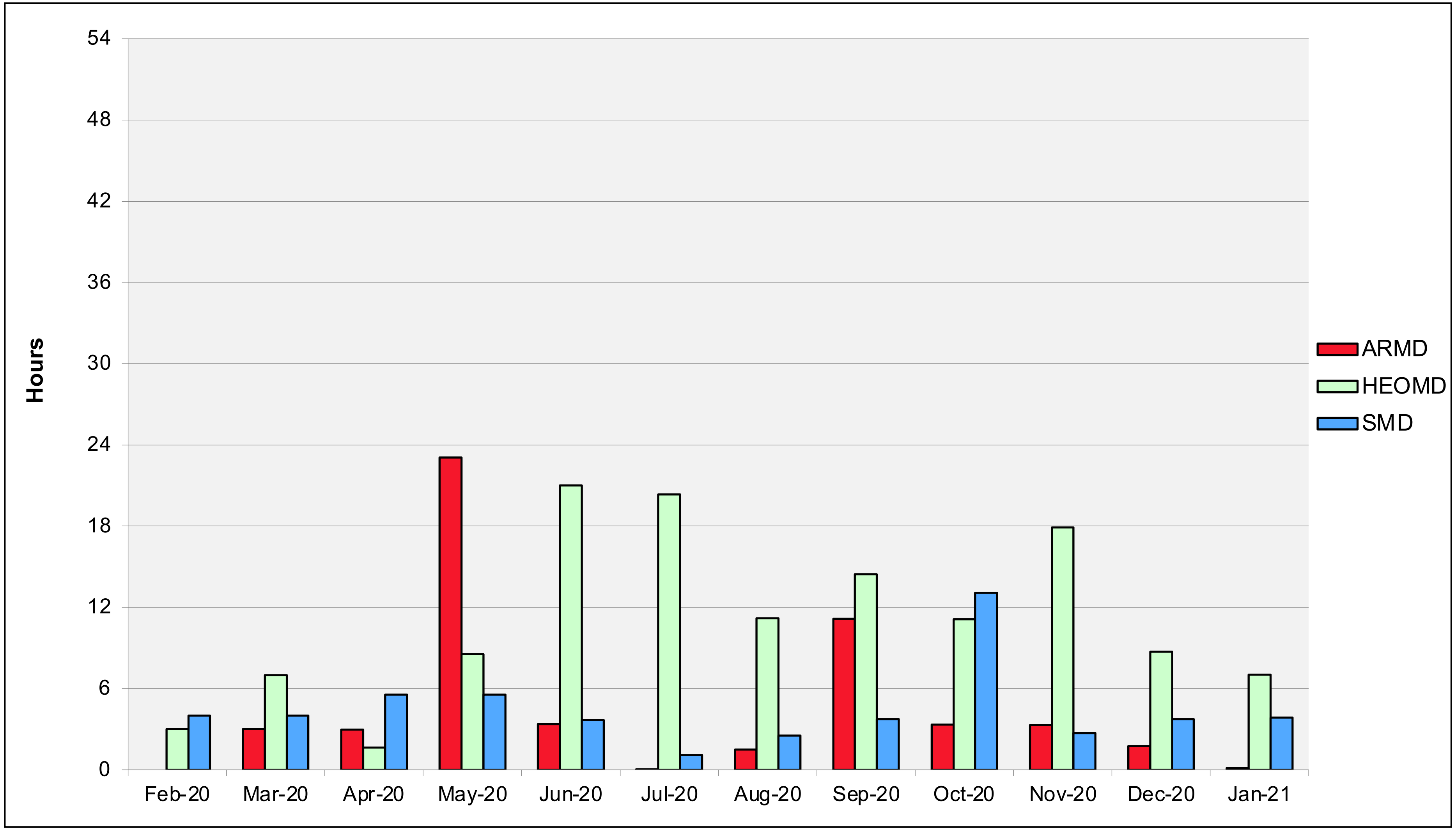
Merope: Monthly Utilization by Job Size



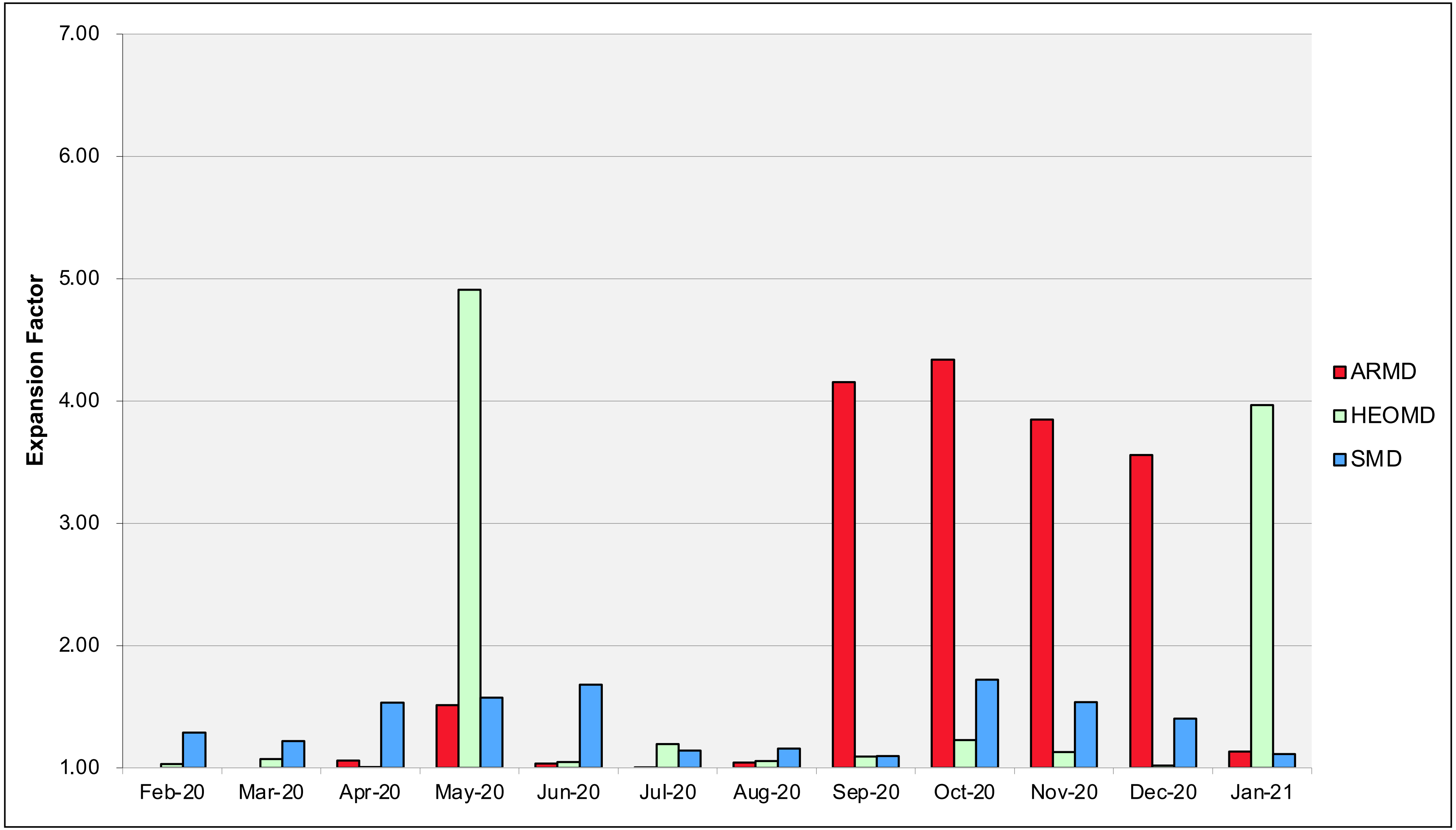
Merope: Monthly Utilization by Size and Length



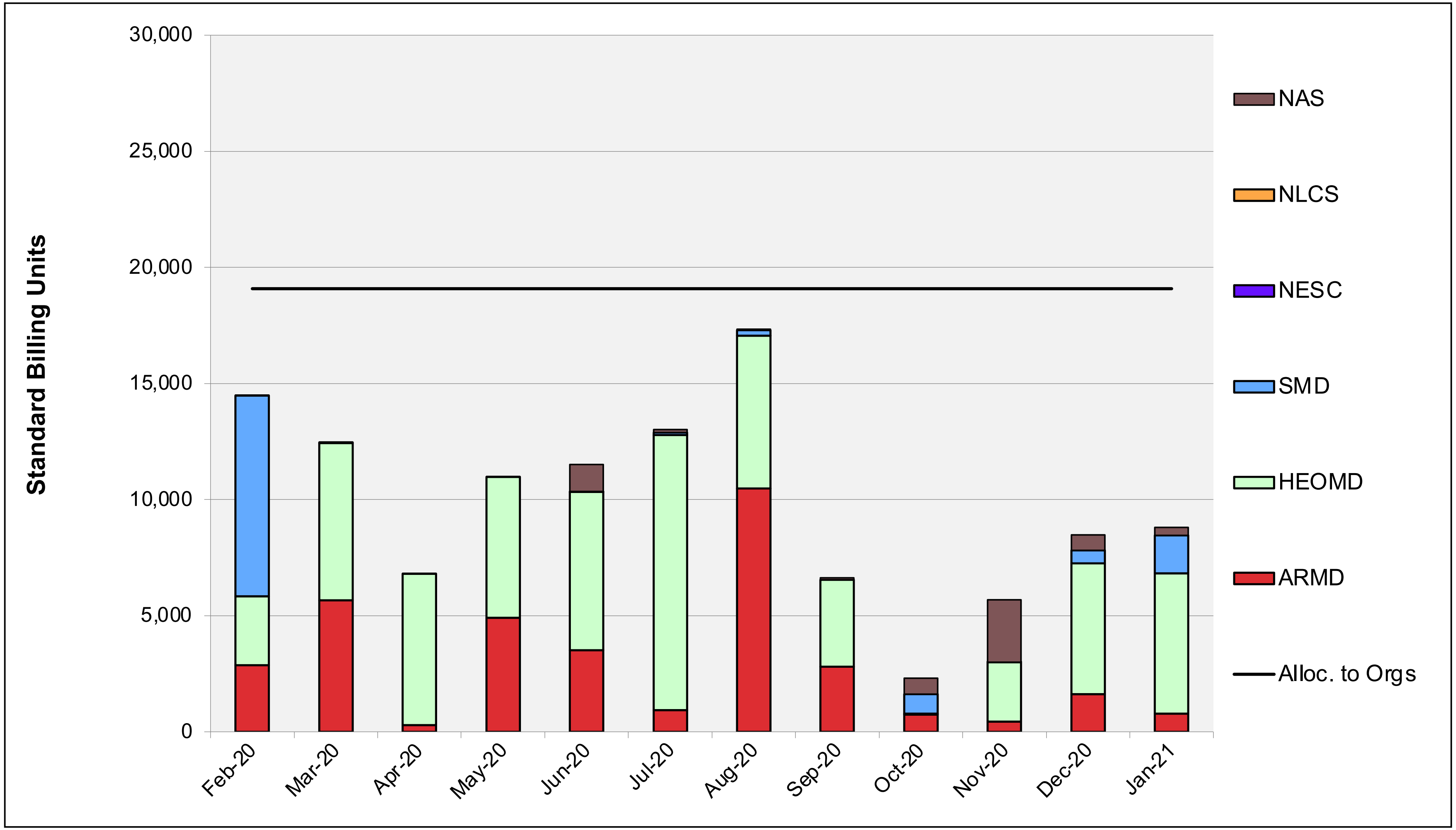
Merope: Average Time to Clear All Jobs



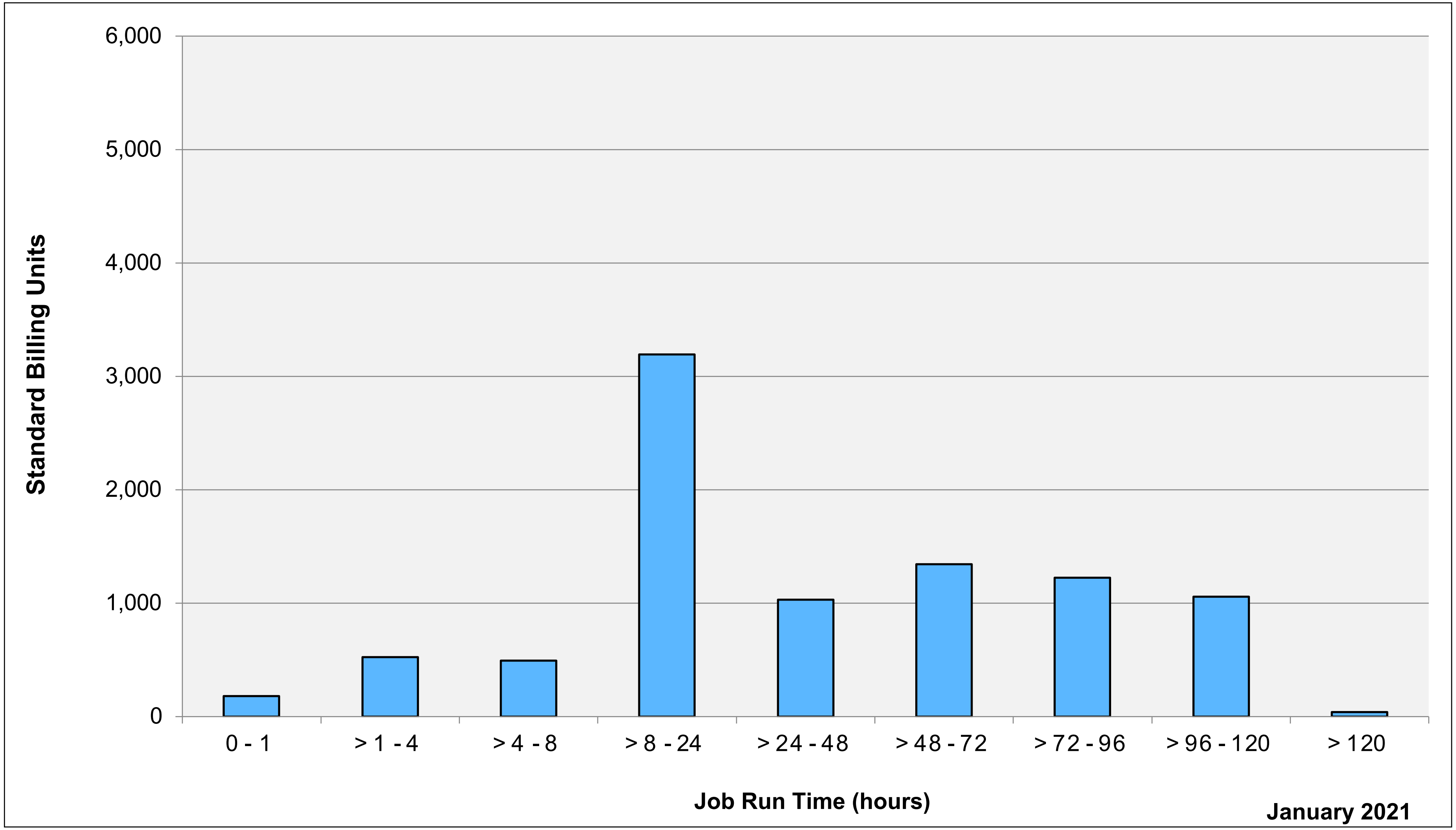
Merope: Average Expansion Factor



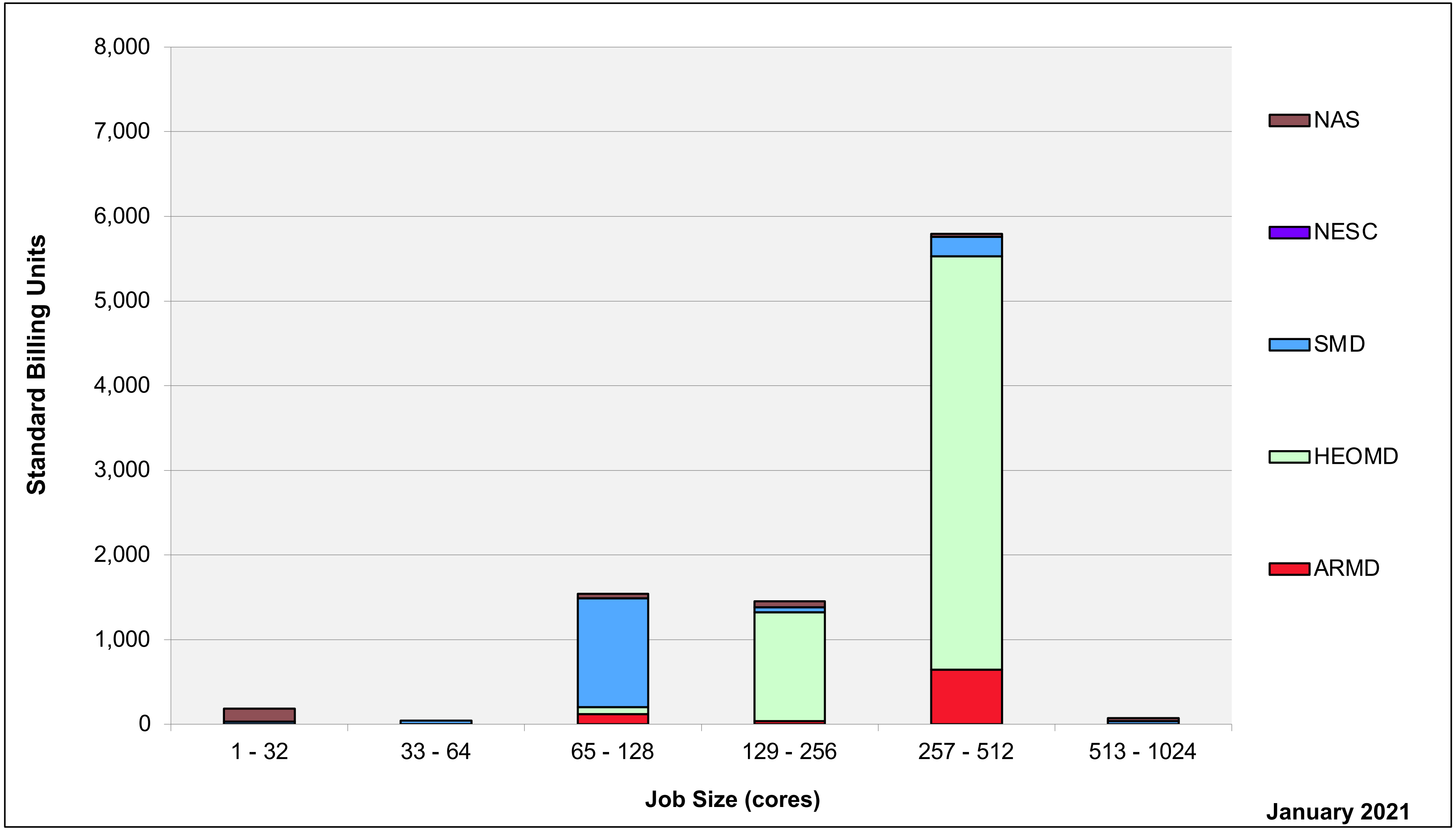
Endeavour: SBUs Reported, Normalized to 30-Day Month



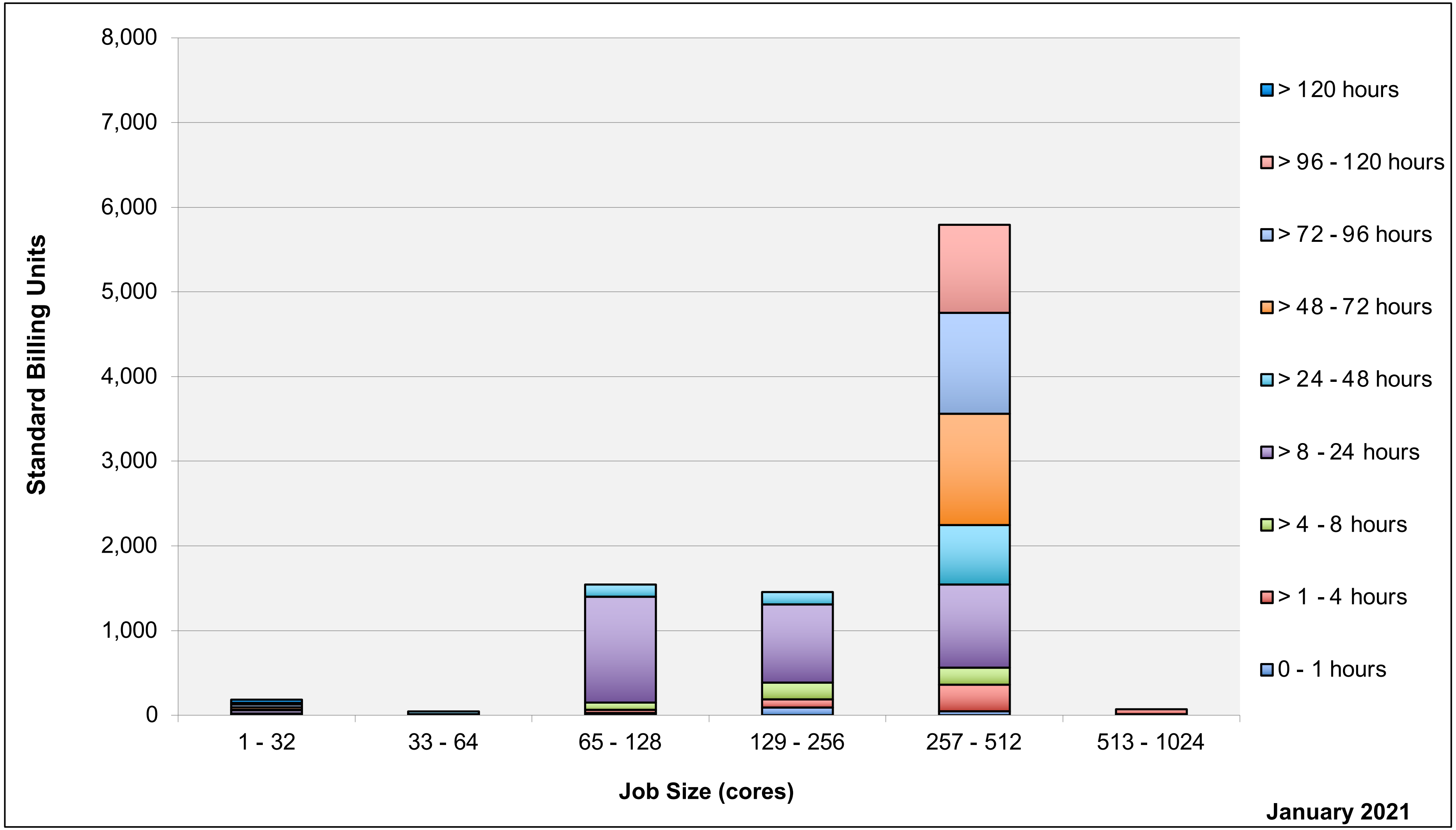
Endeavour: Monthly Utilization by Job Length



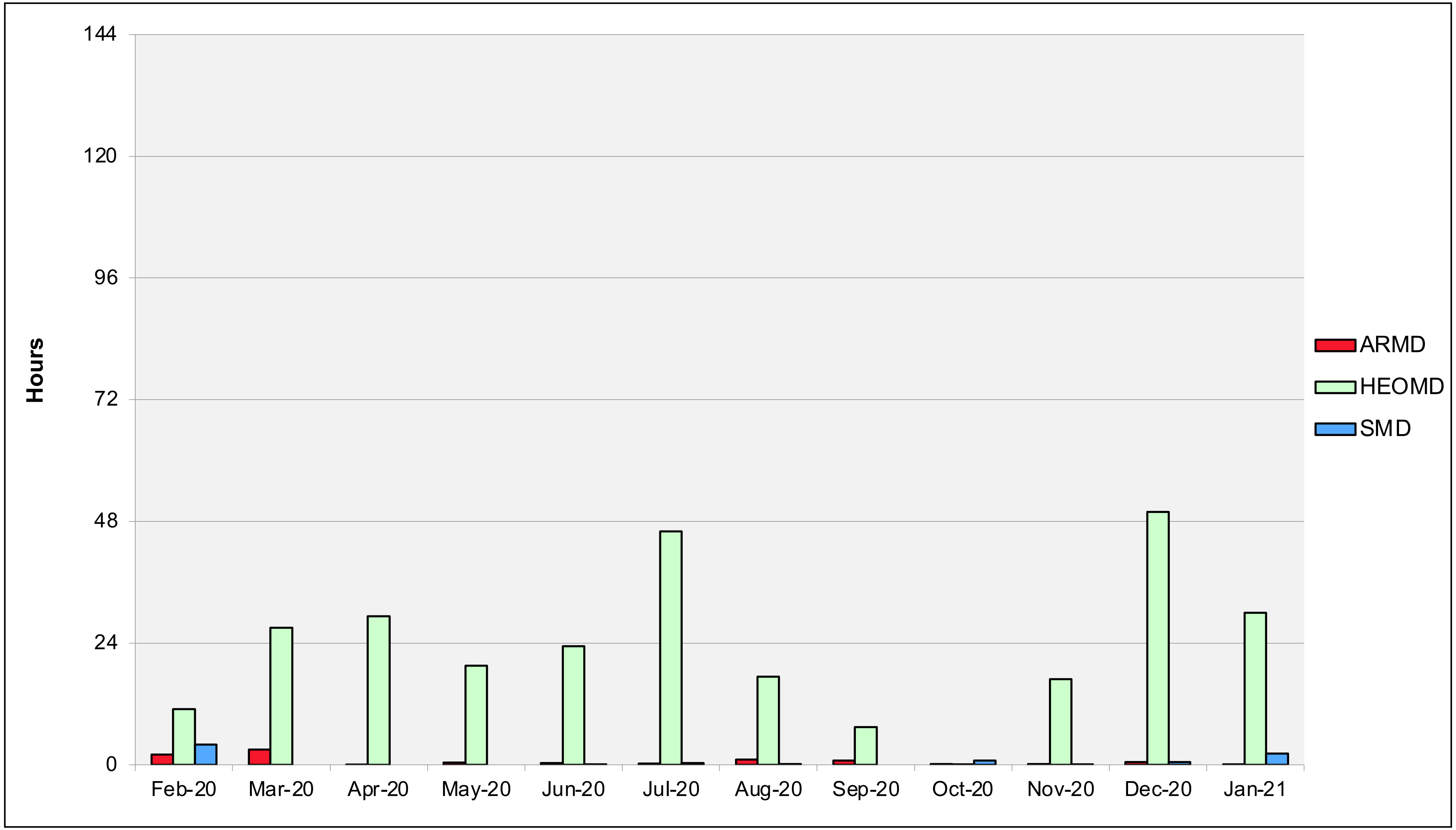
Endeavour: Monthly Utilization by Job Size



Endeavour: Monthly Utilization by Size and Length



Endeavour: Average Time to Clear All Jobs



Endeavour: Average Expansion Factor